Sample name: **M16_octanol**   Experiment start time: **3/1/2018 12:08:09 PM**
Assay name: **pH-metric high logP**   Analyst: **Pion**
Assay ID: **18C-01009**   Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01009_M16_octanol_pH-metric high logP.t3r**

pH-metric Result

logP (XH2 +)   -0.17   ±0.20 (n=50)
logP (neutral XH)   3.04   ±0.01 (n=50)
logP (X -)   -1.62

18C-01009 Points 1 to 31

M16_octanol concentration factor   0.767
Carbonate   0.0840 mM
Acidity error   3.05344 mM

18C-01009 Points 32 to 62

M16_octanol concentration factor   0.794
Carbonate   0.1938 mM
Acidity error   2.68082 mM

18C-01009 Points 63 to 92

M16_octanol concentration factor   0.836
Carbonate   0.2810 mM
Acidity error   2.47693 mM

Warnings and errors
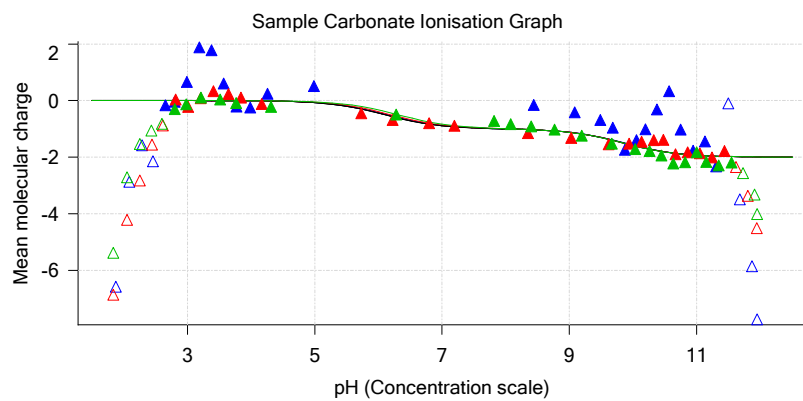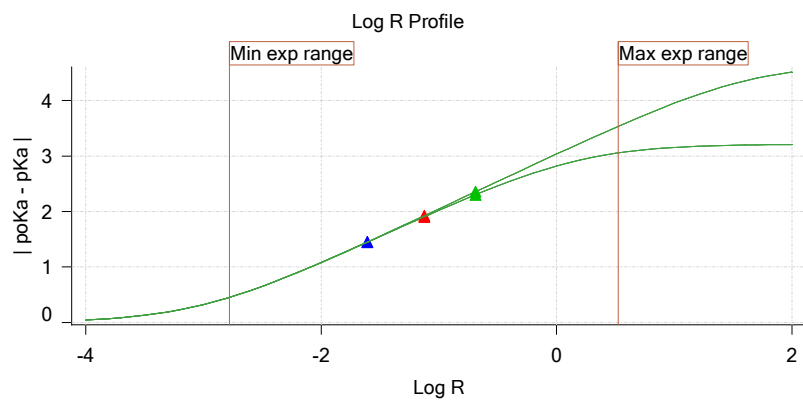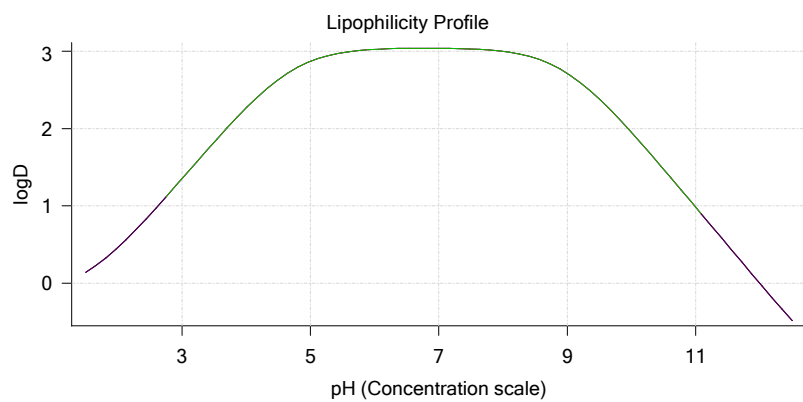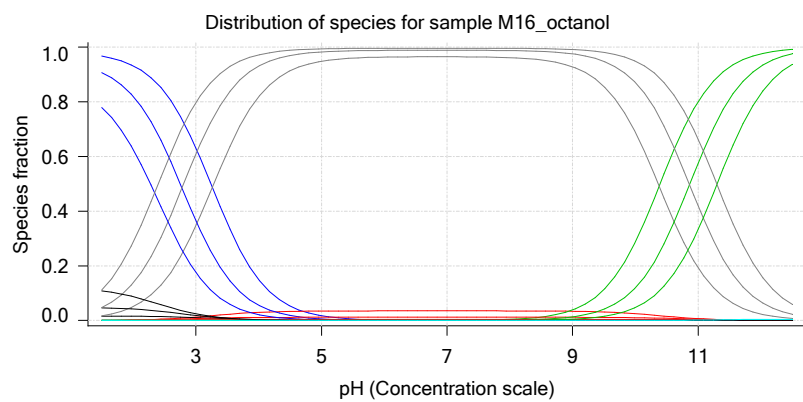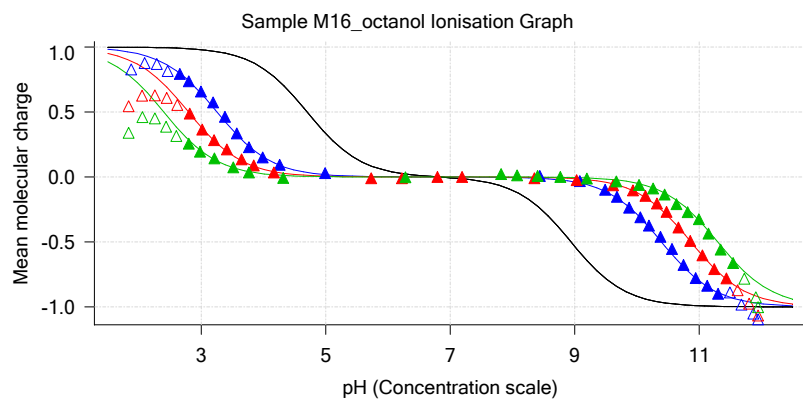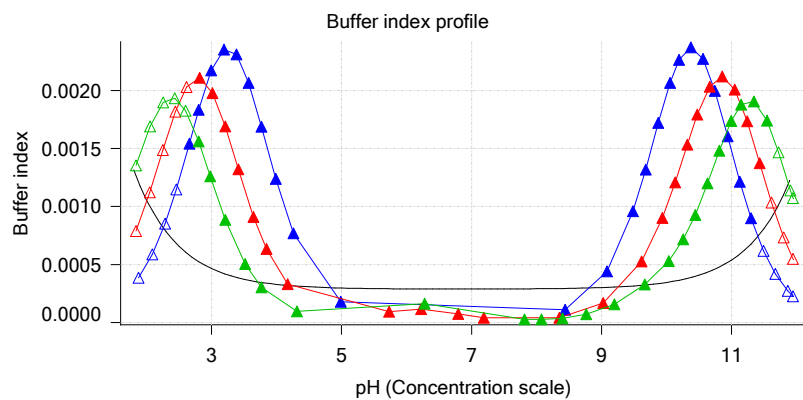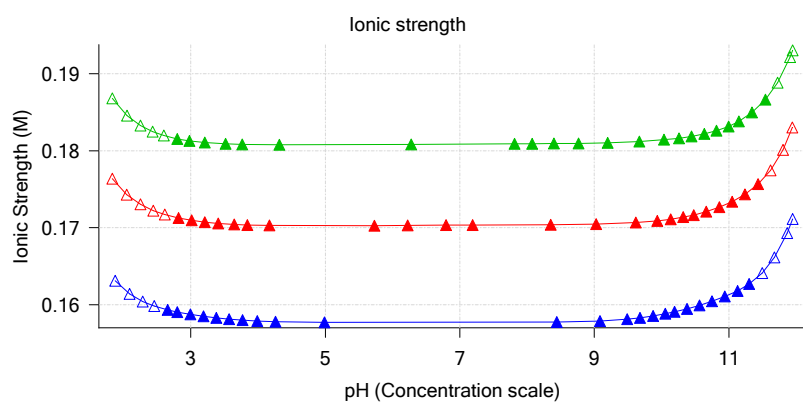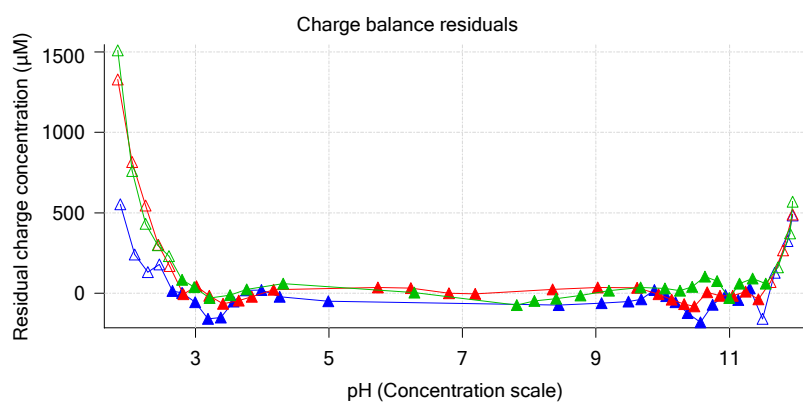
Errors   None
Warnings None

Sample logD and percent species

pH	M16_octanol logD	M16_octanol M16_octanolH2	M16_octanol M16_octanolH	M16_octanol M16_octanol	M16_octanol M16_octanolH2*	M16_octanol M16_octanolH*	M16_octanol M16_octanol*	Comment
1.000	-0.05	52.62 %	0.01 %	0.00 %	35.72 %	11.64 %	0.00 %	
1.200	0.01	49.26 %	0.02 %	0.00 %	33.44 %	17.28 %	0.00 %	Stomach pH
2.000	0.46	25.68 %	0.05 %	0.00 %	17.44 %	56.83 %	0.00 %	
3.000	1.35	4.20 %	0.08 %	0.00 %	2.85 %	92.87 %	0.00 %	
4.000	2.27	0.45 %	0.09 %	0.00 %	0.30 %	99.16 %	0.00 %	
5.000	2.87	0.05 %	0.09 %	0.00 %	0.03 %	99.83 %	0.00 %	
6.000	3.02	0.00 %	0.09 %	0.00 %	0.00 %	99.90 %	0.00 %	
6.500	3.04	0.00 %	0.09 %	0.00 %	0.00 %	99.91 %	0.00 %	
7.000	3.04	0.00 %	0.09 %	0.00 %	0.00 %	99.91 %	0.00 %	
7.400	3.03	0.00 %	0.09 %	0.00 %	0.00 %	99.91 %	0.00 %	Blood pH
8.000	3.00	0.00 %	0.09 %	0.01 %	0.00 %	99.90 %	0.00 %	
9.000	2.71	0.00 %	0.09 %	0.10 %	0.00 %	99.80 %	0.00 %	
10.000	1.95	0.00 %	0.09 %	1.02 %	0.00 %	98.86 %	0.02 %	
11.000	0.98	0.00 %	0.08 %	9.35 %	0.00 %	90.34 %	0.22 %	
12.000	-0.00	0.00 %	0.04 %	50.23 %	0.00 %	48.52 %	1.20 %	

Sample name: **M16_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01009**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01009_M16_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 12:08:09 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Graphs

Charge balance residuals

Ionic strength

Buffer index profile

Sample M16_octanol Ionisation Graph

Distribution of species for sample M16_octanol

Lipophilicity Profile

Log R Profile

Sample Carbonate Ionisation Graph

Sample name: **M16_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01009**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01009_M16_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 12:08:09 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Graphs (continued)

Distribution of species for sample Carbonate

Sample name: **M16_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01009**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01009_M16_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 12:08:09 PM**
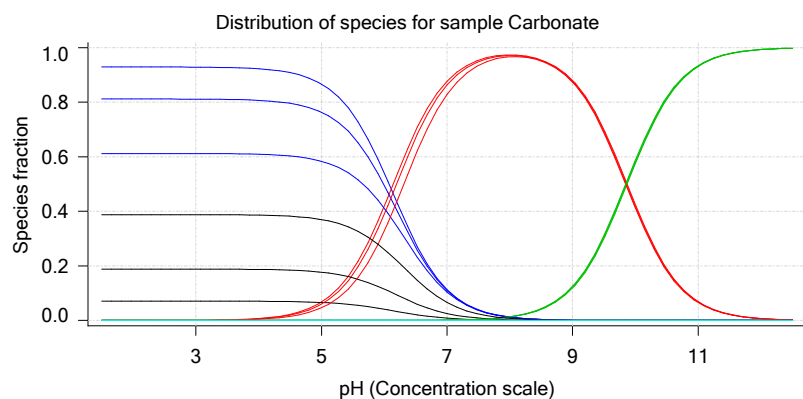Analyst: **Pion**
Instrument ID: **T312060**

pH-metric high logP   Titration 1 of 3   18C-01009 Points 1 to 31

Overall results

RMSD   0.138
Average ionic strength   0.159 M
Average temperature   25.0°C
Partition ratio   0.0247 : 1
Analyte concentration range   4991.2 µM to 5365.1 µM
Total points considered   23 of 31

Warnings and errors

Errors   None
Warnings   Excessive acidity error present

Four-Plus parameters

Alpha   0.130   3/1/2018 12:08:08 PM   C:\Sirius_T3\HCl18B27.t3r
S   0.9970   3/1/2018 12:08:08 PM   C:\Sirius_T3\HCl18B27.t3r
jH   0.8   3/1/2018 12:08:08 PM   C:\Sirius_T3\HCl18B27.t3r
jOH   -0.4   3/1/2018 12:08:08 PM   C:\Sirius_T3\HCl18B27.t3r

Titrants

0.50 M HCl   0.993513   3/1/2018 12:08:08 PM   C:\Sirius_T3\HCl18B27.t3r
0.50 M KOH   0.999845   3/1/2018 12:08:09 PM   C:\Sirius_T3\KOH18B27.t3r

Sample

M16_octanol concentration factor   0.767
Base pKa 1   4.70
Acid pKa 2   8.94
logP (XH2 +)   0.85
logP (neutral XH)   3.08
logP (X -)   -1.62

Sample graphs

Ionisation of sample M16_octanol

Distribution of species for sample M16_octanol

Sample name: **M16_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01009**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01009_M16_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 12:08:09 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Sample graphs (continued)

Lipophilicity Profile

Sample logD and percent species

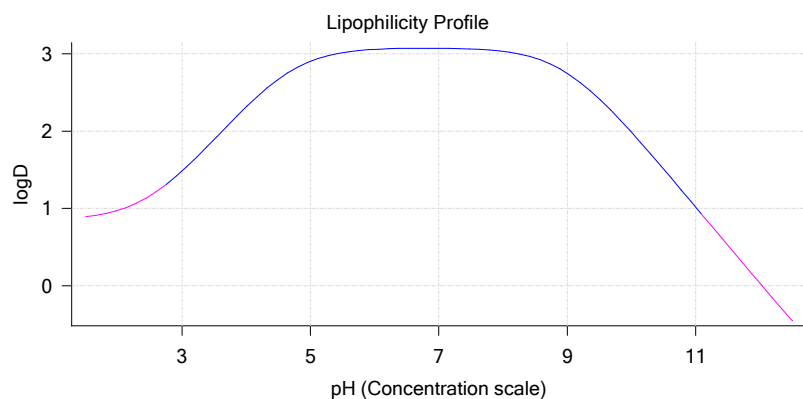| pH	M16_octanol logD	M16_octanol M16_octanolH2	M16_octanol M16_octanolH	M16_octanol M16_octanol	M16_octanol M16_octanolH2*	M16_octanol M16_octanolH*	M16_octanol M16_octanol*	Comment
1.000	0.86	84.71 %	0.02 %	0.00 %	14.77 %	0.50 %	0.00 %	
1.200	0.87	84.45 %	0.03 %	0.00 %	14.73 %	0.79 %	0.00 %	Stomach pH
2.000	0.97	80.93 %	0.16 %	0.00 %	14.12 %	4.80 %	0.00 %	
3.000	1.48	55.95 %	1.12 %	0.00 %	9.76 %	33.17 %	0.00 %	
4.000	2.31	13.69 %	2.73 %	0.00 %	2.39 %	81.18 %	0.00 %	
5.000	2.90	1.60 %	3.19 %	0.00 %	0.28 %	94.92 %	0.00 %	
6.000	3.06	0.16 %	3.25 %	0.00 %	0.03 %	96.56 %	0.00 %	
6.500	3.07	0.05 %	3.25 %	0.01 %	0.01 %	96.67 %	0.00 %	
7.000	3.07	0.02 %	3.25 %	0.04 %	0.00 %	96.69 %	0.00 %	
7.400	3.07	0.01 %	3.25 %	0.09 %	0.00 %	96.65 %	0.00 %	Blood pH
8.000	3.03	0.00 %	3.24 %	0.37 %	0.00 %	96.38 %	0.00 %	
9.000	2.75	0.00 %	3.14 %	3.60 %	0.00 %	93.26 %	0.00 %	
10.000	1.98	0.00 %	2.37 %	27.21 %	0.00 %	70.41 %	0.02 %	
11.000	1.02	0.00 %	0.69 %	78.86 %	0.00 %	20.41 %	0.05 %	
12.000	0.03	0.00 %	0.08 %	97.34 %	0.00 %	2.52 %	0.06 %	

Carbonate and acidity

Carbonate   0.084 mM
Acidity error   3.053 mM

Other graphs

Assay progress

Titration graph

Sample name: **M16_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01009**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01009_M16_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 12:08:09 PM**
Analyst: **Pion**
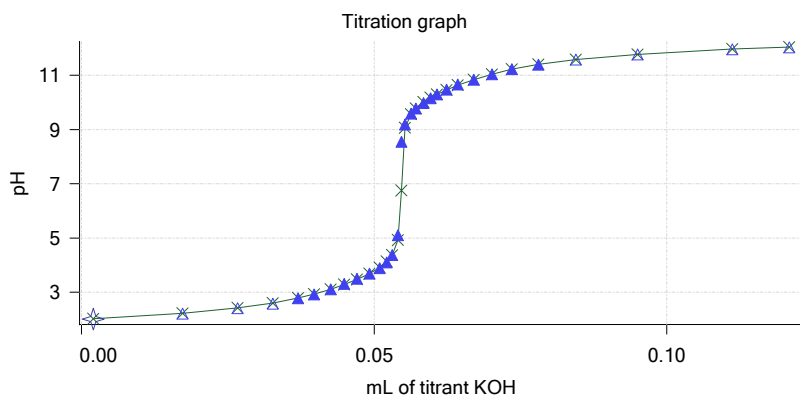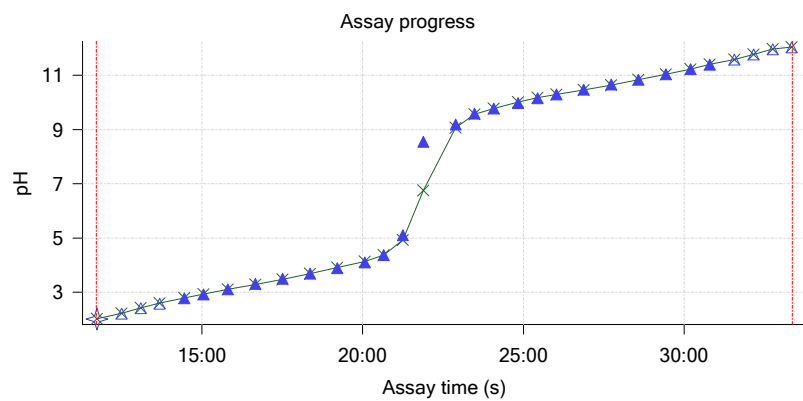Instrument ID: **T312060**

Other graphs (continued)

Charge balance residuals

Buffer index profile
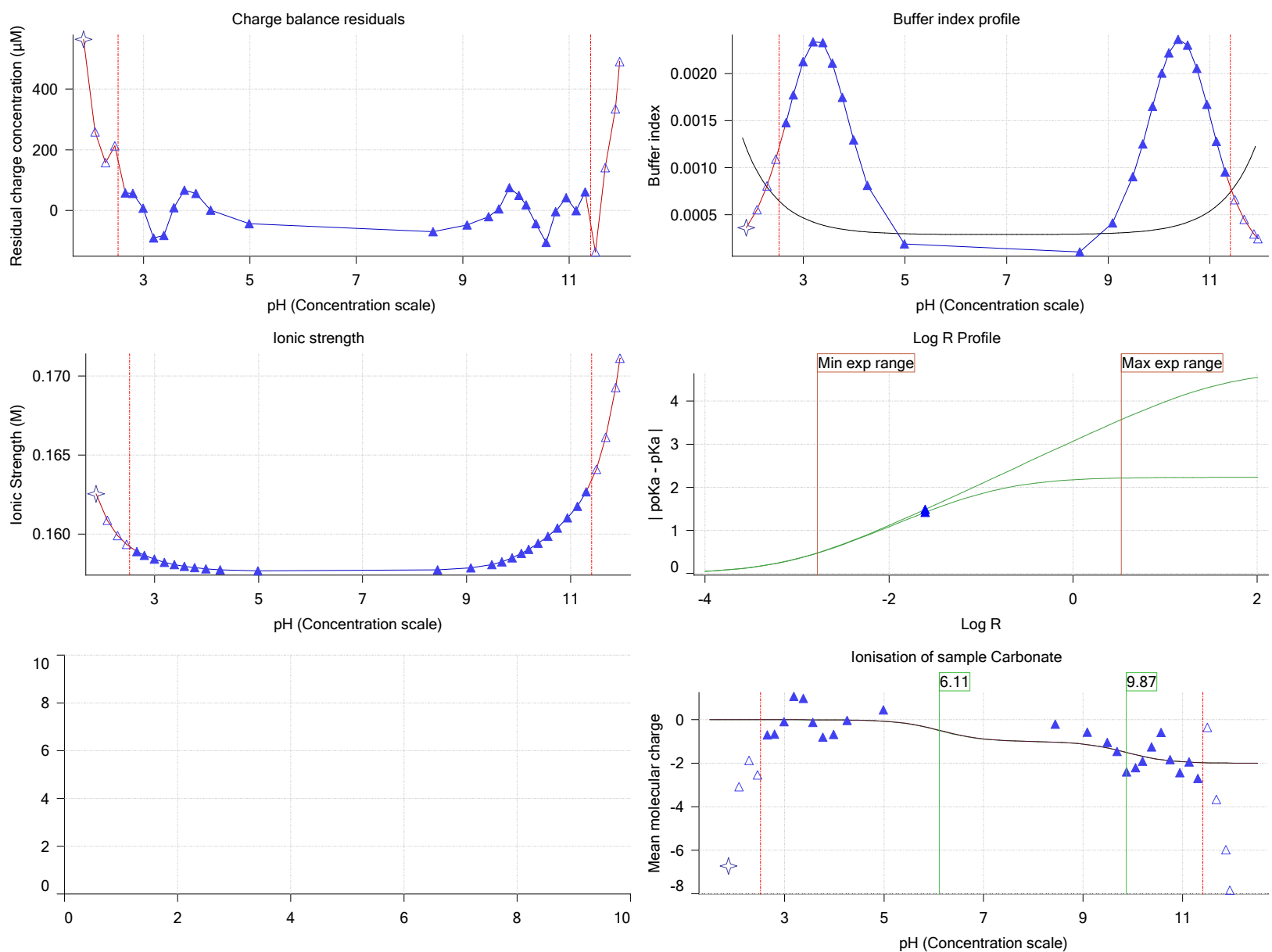
Ionic strength

Log R Profile

Ionisation of sample Carbonate

Sample name: **M16_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01009**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01009_M16_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 12:08:09 PM**
Analyst: **Pion**
Instrument ID: **T312060**

pH-metric high logP   Titration 2 of 3   18C-01009 Points 32 to 62

Overall results

RMSD   0.147
Average ionic strength   0.171 M
Average temperature   25.0°C
Partition ratio   0.0751 : 1
Analyte concentration range   4115.3 µM to 4404.0 µM
Total points considered   23 of 31

Warnings and errors

Errors   None
Warnings   Excessive acidity error present

Four-Plus parameters

Alpha   0.130   3/1/2018 12:08:08 PM   C:\Sirius_T3\HCl18B27.t3r
S   0.9970   3/1/2018 12:08:08 PM   C:\Sirius_T3\HCl18B27.t3r
jH   0.8   3/1/2018 12:08:08 PM   C:\Sirius_T3\HCl18B27.t3r
jOH   -0.4   3/1/2018 12:08:08 PM   C:\Sirius_T3\HCl18B27.t3r

Titrants

0.50 M HCl   0.993513   3/1/2018 12:08:08 PM   C:\Sirius_T3\HCl18B27.t3r
0.50 M KOH   0.999845   3/1/2018 12:08:09 PM   C:\Sirius_T3\KOH18B27.t3r

Sample

M16_octanol concentration factor   0.794
Base pKa 1   4.70
Acid pKa 2   8.94
logP (XH2 +)   0.03
logP (neutral XH)   3.06
logP (X -)   -1.62

Sample graphs

Ionisation of sample M16_octanol

Distribution of species for sample M16_octanol

Sample name: **M16_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01009**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01009_M16_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 12:08:09 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Sample graphs (continued)

Lipophilicity Profile

Sample logD and percent species

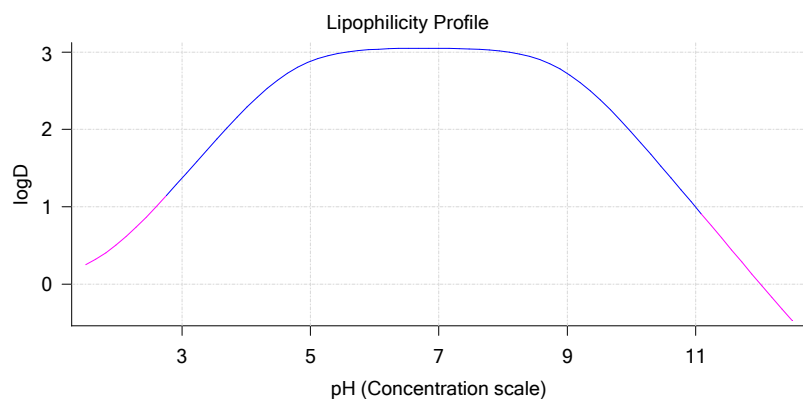| pH	M16_octanol logD	M16_octanol M16_octanolH2	M16_octanol M16_octanolH	M16_octanol M16_octanol	M16_octanol M16_octanolH2*	M16_octanol M16_octanolH*	M16_octanol M16_octanol*	Comment
1.000	0.11	91.17 %	0.02 %	0.00 %	7.26 %	1.55 %	0.00 %	
1.200	0.15	90.33 %	0.03 %	0.00 %	7.20 %	2.44 %	0.00 %	Stomach pH
2.000	0.52	79.86 %	0.16 %	0.00 %	6.36 %	13.62 %	0.00 %	
3.000	1.37	35.65 %	0.71 %	0.00 %	2.84 %	60.80 %	0.00 %	
4.000	2.28	5.45 %	1.09 %	0.00 %	0.43 %	93.02 %	0.00 %	
5.000	2.88	0.58 %	1.15 %	0.00 %	0.05 %	98.23 %	0.00 %	
6.000	3.03	0.06 %	1.16 %	0.00 %	0.00 %	98.78 %	0.00 %	
6.500	3.05	0.02 %	1.16 %	0.00 %	0.00 %	98.82 %	0.00 %	
7.000	3.05	0.01 %	1.16 %	0.01 %	0.00 %	98.82 %	0.00 %	
7.400	3.04	0.00 %	1.16 %	0.03 %	0.00 %	98.81 %	0.00 %	Blood pH
8.000	3.01	0.00 %	1.15 %	0.13 %	0.00 %	98.71 %	0.00 %	
9.000	2.72	0.00 %	1.14 %	1.31 %	0.00 %	97.55 %	0.00 %	
10.000	1.96	0.00 %	1.02 %	11.72 %	0.00 %	87.24 %	0.02 %	
11.000	0.99	0.00 %	0.50 %	56.98 %	0.00 %	42.42 %	0.10 %	
12.000	0.01	0.00 %	0.08 %	92.84 %	0.00 %	6.91 %	0.17 %	

Carbonate and acidity

Carbonate   0.194 mM
Acidity error   2.681 mM

Other graphs

Assay progress

Titration graph

Sample name: **M16_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01009**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01009_M16_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 12:08:09 PM**
Analyst: **Pion**
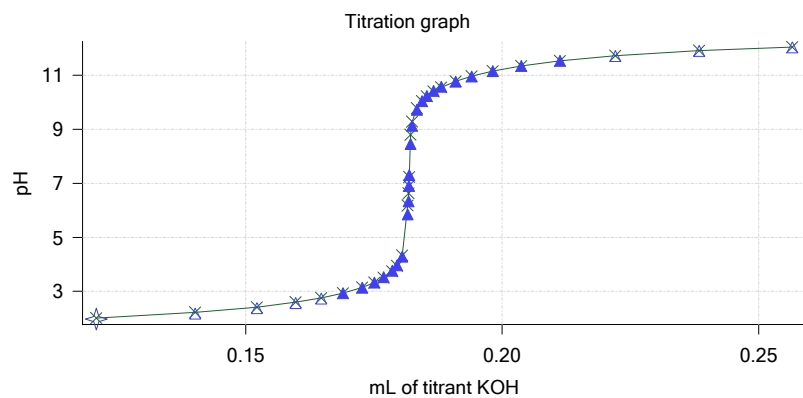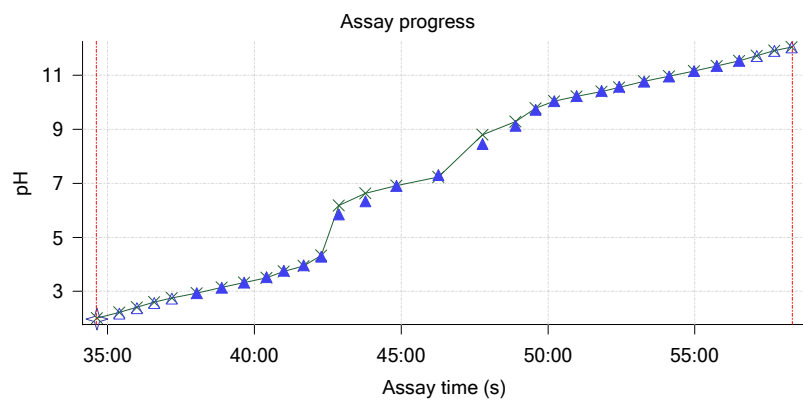Instrument ID: **T312060**

Other graphs (continued)

Charge balance residuals

Buffer index profile

Ionic strength

Log R Profile

Ionisation of sample Carbonate
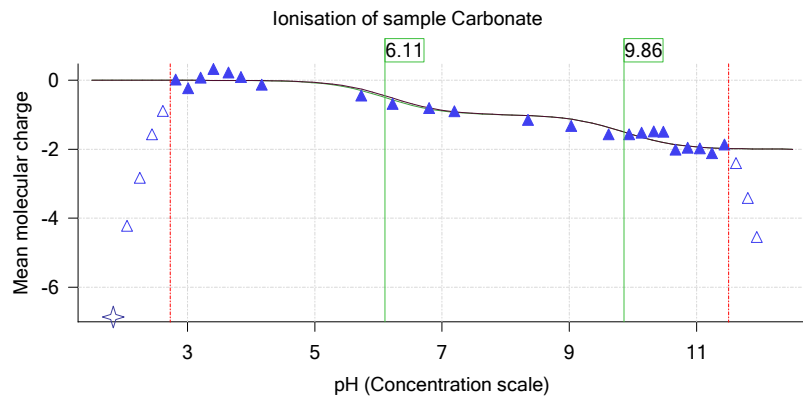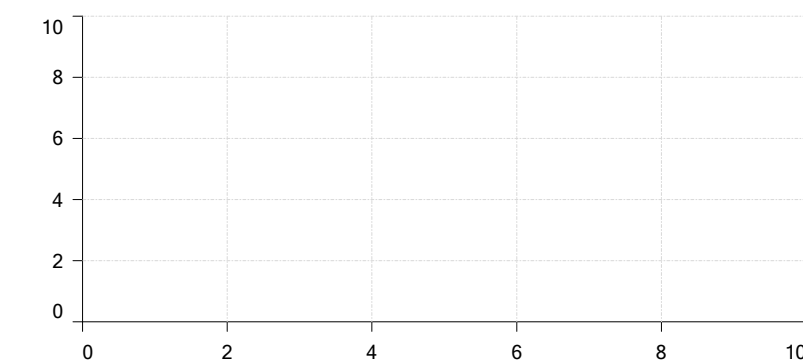
Sample name: **M16_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01009**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01009_M16_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 12:08:09 PM**
Analyst: **Pion**
Instrument ID: **T312060**

pH-metric high logP   Titration 3 of 3   18C-01009 Points 63 to 92

Overall results

RMSD   0.627
Average ionic strength   0.182 M
Average temperature   25.0°C
Partition ratio   0.2052 : 1
Analyte concentration range   3198.3 µM to 3391.8 µM
Total points considered   22 of 30

Warnings and errors

Errors   None
Warnings   One or more logP values out of range
           Excessive acidity error present

Four-Plus parameters

Alpha 0.130   3/1/2018 12:08:08 PM   C:\Sirius_T3\HCl18B27.t3r
S   0.9970 3/1/2018 12:08:08 PM   C:\Sirius_T3\HCl18B27.t3r
jH   0.8   3/1/2018 12:08:08 PM   C:\Sirius_T3\HCl18B27.t3r
jOH   -0.4   3/1/2018 12:08:08 PM   C:\Sirius_T3\HCl18B27.t3r

Titrants

0.50 M HCl   0.993513   3/1/2018 12:08:08 PM   C:\Sirius_T3\HCl18B27.t3r
0.50 M KOH   0.999845   3/1/2018 12:08:09 PM   C:\Sirius_T3\KOH18B27.t3r

Sample

M16_octanol concentration factor   0.836
Base pKa 1   4.70
Acid pKa 2   8.94
logP (XH2 +)   -5.10
logP (neutral XH)   3.01
logP (X -)   -1.62

Sample graphs

Ionisation of sample M16_octanol

Distribution of species for sample M16_octanol
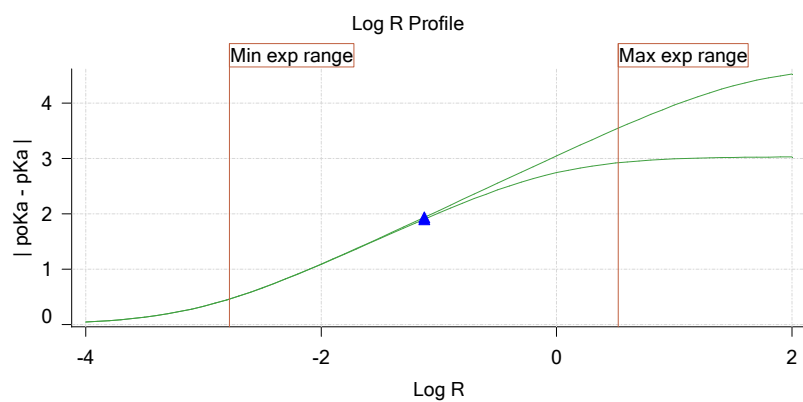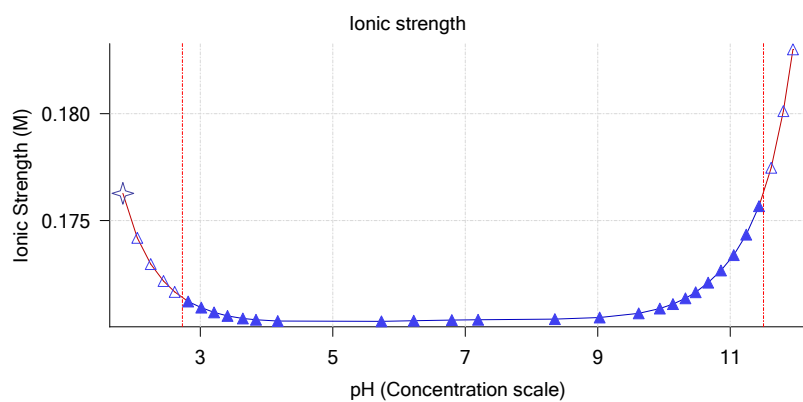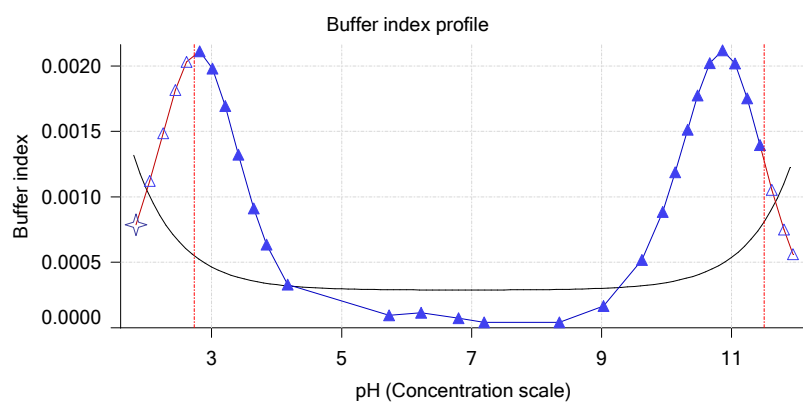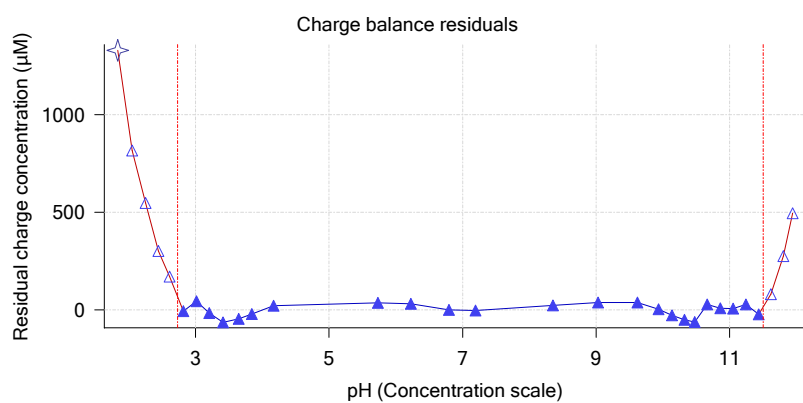
Sample name: **M16_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01009**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01009_M16_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 12:08:09 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Sample graphs (continued)

Lipophilicity Profile
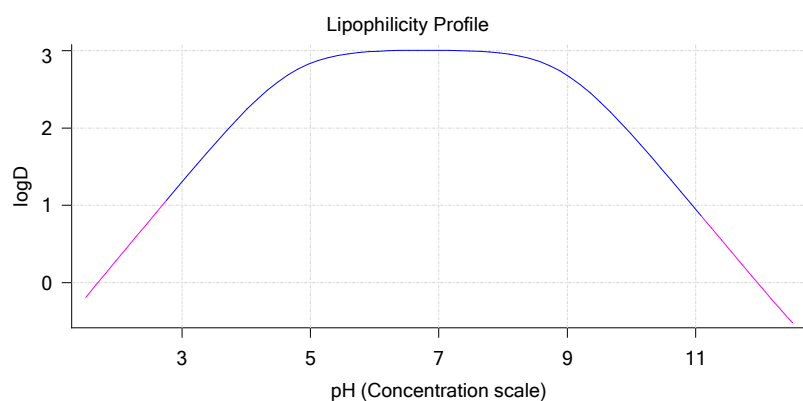
Sample logD and percent species

pH	M16_octanol logD	M16_octanol M16_octanolH2	M16_octanol M16_octanolH	M16_octanol M16_octanol	M16_octanol M16_octanolH2*	M16_octanol M16_octanolH*	M16_octanol M16_octanol*	Comment
1.000	-0.69	95.95 %	0.02 %	0.00 %	0.00 %	4.03 %	0.00 %	
1.200	-0.49	93.73 %	0.03 %	0.00 %	0.00 %	6.24 %	0.00 %	Stomach pH
2.000	0.31	70.32 %	0.14 %	0.00 %	0.00 %	29.54 %	0.00 %	
3.000	1.30	19.16 %	0.38 %	0.00 %	0.00 %	80.46 %	0.00 %	
4.000	2.23	2.31 %	0.46 %	0.00 %	0.00 %	97.22 %	0.00 %	
5.000	2.83	0.24 %	0.47 %	0.00 %	0.00 %	99.29 %	0.00 %	
6.000	2.99	0.02 %	0.47 %	0.00 %	0.00 %	99.50 %	0.00 %	
6.500	3.00	0.01 %	0.47 %	0.00 %	0.00 %	99.52 %	0.00 %	
7.000	3.00	0.00 %	0.47 %	0.01 %	0.00 %	99.52 %	0.00 %	
7.400	3.00	0.00 %	0.47 %	0.01 %	0.00 %	99.51 %	0.00 %	Blood pH
8.000	2.96	0.00 %	0.47 %	0.05 %	0.00 %	99.47 %	0.00 %	
9.000	2.68	0.00 %	0.47 %	0.54 %	0.00 %	98.99 %	0.00 %	
10.000	1.92	0.00 %	0.45 %	5.15 %	0.00 %	94.38 %	0.03 %	
11.000	0.95	0.00 %	0.31 %	35.12 %	0.00 %	64.40 %	0.17 %	
12.000	-0.04	0.00 %	0.07 %	84.09 %	0.00 %	15.42 %	0.41 %	

Carbonate and acidity

Carbonate   0.281 mM
Acidity error   2.477 mM

Other graphs

Assay progress

Titration graph

Sample name: **M16_octanol**   Experiment start time: **3/1/2018 12:08:09 PM**

Assay name: **pH-metric high logP**   Analyst: **Pion**

Assay ID: **18C-01009**   Instrument ID: **T312060**

Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01009_M16_octanol_pH-metric high logP.t3r**

Other graphs (continued)

Charge balance residuals

Buffer index profile

Ionic strength

Log R Profile

Ionisation of sample Carbonate
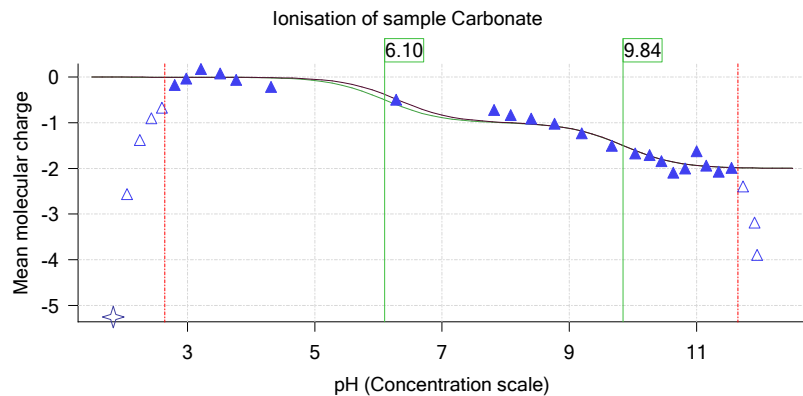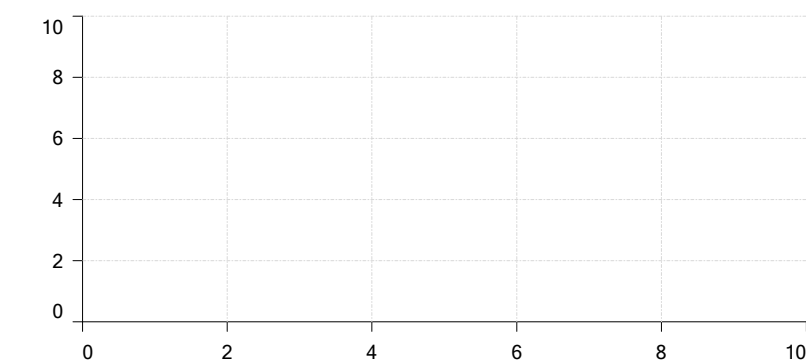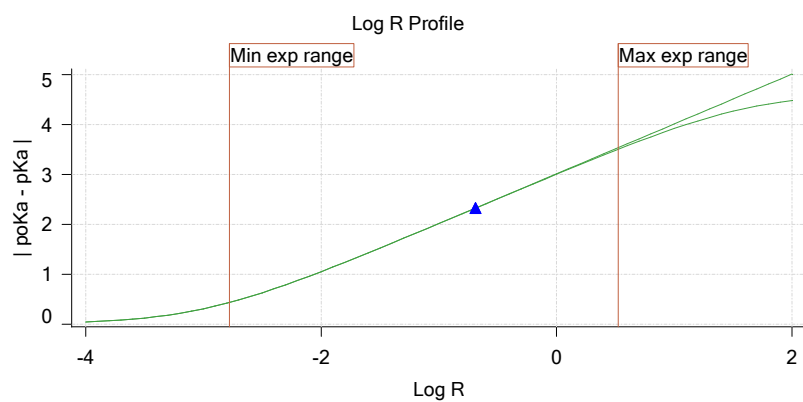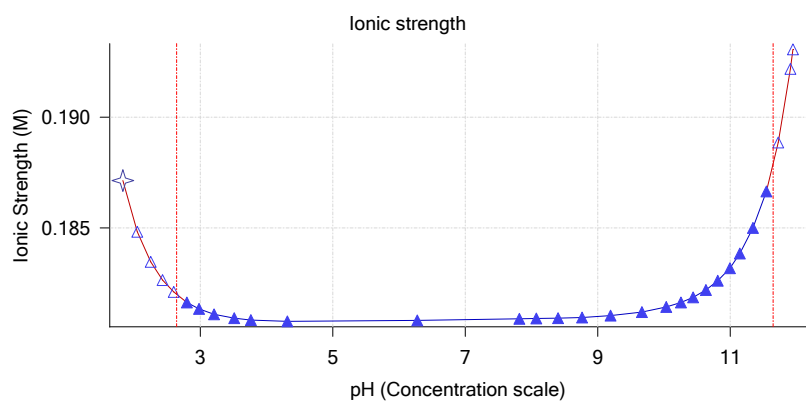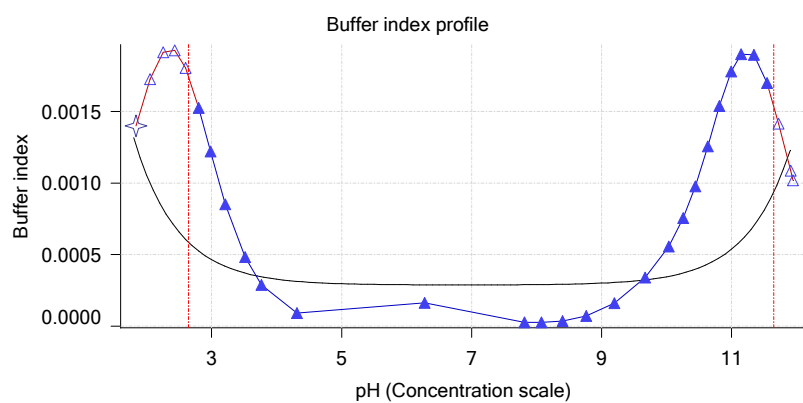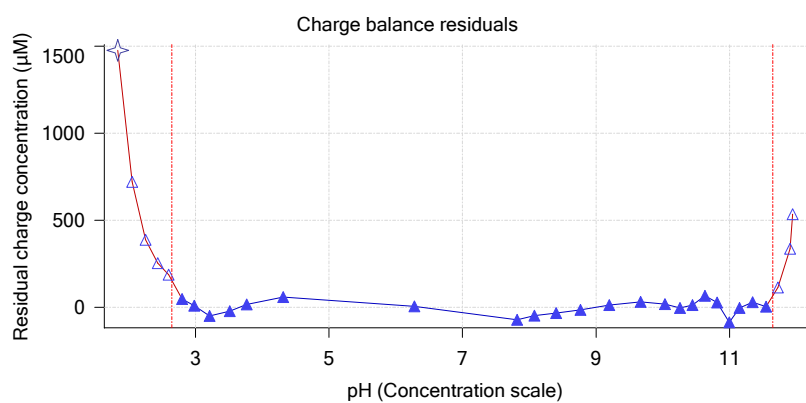
Sample name: **M16_octanol**　　　　　　　　Experiment start time: **3/1/2018 12:08:09 PM**
Assay name: **pH-metric high logP**　　　　　　Analyst: **Pion**
Assay ID: **18C-01009**　　　　　　　　　　Instrument ID: **T312060**
Filename:　　**C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01009_M16_octanol_pH-metric high logP.t3r**

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	M16_octanol	2/27/2018 6:14:13 PM	User entered value
Sample by	Weight		Default value
Sample weight	0.001790 g	2/28/2018 4:25:54 PM	User entered value
Formula weight	210.23 g/mol	2/27/2018 5:08:55 PM	User entered value
Solubility	Unknown		Default value
Molecular weight	210.23	2/27/2018 5:08:55 PM	User entered value
Individual pKa ionic environments	No		Default value
Number of pKas	2	2/27/2018 5:08:55 PM	User entered value
Sample is a	Ampholyte	2/27/2018 5:08:55 PM	User entered value
pKa 1	4.70	2/27/2018 5:08:55 PM	User entered value
Type	Base	2/27/2018 5:08:55 PM	User entered value
pKa 2	8.94	2/27/2018 5:08:55 PM	User entered value
Type	Acid	2/27/2018 5:08:55 PM	User entered value
logp (XH2 +)	-0.97	2/27/2018 5:09:30 PM	User entered value
logP (neutral XH)	1.47	2/27/2018 5:09:44 PM	User entered value
logP (X -)	-1.62	2/27/2018 5:09:50 PM	User entered value

Events

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
8:39.5	Initial pH = 3.74									
11:44.1	Data point 1	1.50000 mL	0.04499 mL	0.00202 mL	0.04000 mL	2.009	-0.00786	0.25633	0.00077	10.0 s
12:30.3	Data point 2	1.50000 mL	0.04499 mL	0.01726 mL	0.04000 mL	2.218	-0.00029	0.00763	0.00016	10.0 s
13:06.0	Data point 3	1.50000 mL	0.04499 mL	0.02667 mL	0.04000 mL	2.413	-0.00594	0.13958	0.00079	10.0 s
13:41.5	Data point 4	1.50000 mL	0.04499 mL	0.03269 mL	0.04000 mL	2.584	-0.00084	0.06954	0.00016	10.0 s
14:27.4	Data point 5	1.50000 mL	0.04499 mL	0.03702 mL	0.04000 mL	2.780	-0.00378	0.06388	0.00074	10.0 s
15:02.9	Data point 6	1.50000 mL	0.04499 mL	0.03972 mL	0.04000 mL	2.922	-0.00866	0.21191	0.00093	10.0 s
15:48.8	Data point 7	1.50000 mL	0.04499 mL	0.04259 mL	0.04000 mL	3.115	-0.00483	0.80380	0.00027	10.0 s
16:39.8	Data point 8	1.50000 mL	0.04499 mL	0.04485 mL	0.04000 mL	3.309	-0.00755	0.21309	0.00081	10.0 s
17:30.8	Data point 9	1.50000 mL	0.04499 mL	0.04706 mL	0.04000 mL	3.501	-0.00612	0.78470	0.00034	10.0 s
18:21.9	Data point 10	1.50000 mL	0.04499 mL	0.04920 mL	0.04000 mL	3.691	-0.00337	0.03338	0.00091	10.0 s
19:12.8	Data point 11	1.50000 mL	0.04499 mL	0.05092 mL	0.04000 mL	3.887	-0.00649	0.12208	0.00092	10.0 s
20:03.7	Data point 12	1.50000 mL	0.04499 mL	0.05216 mL	0.04000 mL	4.105	-0.01178	0.65123	0.00072	10.0 s
20:39.2	Data point 13	1.50000 mL	0.04499 mL	0.05306 mL	0.04000 mL	4.377	-0.01852	0.90826	0.00096	10.5 s
21:15.1	Data point 14	1.50000 mL	0.04499 mL	0.05407 mL	0.04000 mL	5.103	-0.01578	0.79081	0.00088	13.0 s
21:53.5	Data point 15	1.50000 mL	0.04499 mL	0.05468 mL	0.04000 mL	8.545	-0.01967	0.99135	0.00098	34.5 s
22:53.5	Data point 16	1.50000 mL	0.04499 mL	0.05527 mL	0.04000 mL	9.186	-0.01692	0.94412	0.00086	10.0 s
23:28.9	Data point 17	1.50000 mL	0.04499 mL	0.05628 mL	0.04000 mL	9.588	-0.01207	0.94821	0.00061	10.0 s
24:04.3	Data point 18	1.50000 mL	0.04499 mL	0.05713 mL	0.04000 mL	9.780	-0.01206	0.54950	0.00080	10.0 s
24:50.2	Data point 19	1.50000 mL	0.04499 mL	0.05842 mL	0.04000 mL	9.975	-0.00092	0.02620	0.00028	10.5 s
25:26.2	Data point 20	1.50000 mL	0.04499 mL	0.05962 mL	0.04000 mL	10.154	-0.00816	0.82899	0.00044	10.0 s
26:01.6	Data point 21	1.50000 mL	0.04499 mL	0.06070 mL	0.04000 mL	10.292	-0.01383	0.62163	0.00087	10.0 s
26:52.5	Data point 22	1.50000 mL	0.04499 mL	0.06235 mL	0.04000 mL	10.475	-0.00623	0.21568	0.00066	10.0 s
27:43.4	Data point 23	1.50000 mL	0.04499 mL	0.06430 mL	0.04000 mL	10.663	-0.01087	0.60836	0.00069	10.0 s
28:34.5	Data point 24	1.50000 mL	0.04499 mL	0.06700 mL	0.04000 mL	10.845	0.00564	0.16265	0.00069	10.5 s
29:26.1	Data point 25	1.50000 mL	0.04499 mL	0.07013 mL	0.04000 mL	11.038	-0.00670	0.84026	0.00036	10.0 s
30:12.0	Data point 26	1.50000 mL	0.04499 mL	0.07354 mL	0.04000 mL	11.226	-0.00717	0.22192	0.00075	10.0 s
30:47.5	Data point 27	1.50000 mL	0.04499 mL	0.07806 mL	0.04000 mL	11.397	0.00185	0.09507	0.00030	10.0 s
31:33.5	Data point 28	1.50000 mL	0.04499 mL	0.08443 mL	0.04000 mL	11.589	-0.00034	0.00072	0.00063	10.0 s
32:09.1	Data point 29	1.50000 mL	0.04499 mL	0.09501 mL	0.04000 mL	11.769	-0.00357	0.09765	0.00056	10.0 s
32:45.0	Data point 30	1.50000 mL	0.04499 mL	0.11117 mL	0.04000 mL	11.958	0.00119	0.00998	0.00059	10.0 s
33:20.6	Data point 31	1.50000 mL	0.04499 mL	0.12091 mL	0.04000 mL	12.036	0.00213	0.35467	0.00018	10.0 s
34:38.0	Data point 32	1.50000 mL	0.17241 mL	0.12091 mL	0.14000 mL	1.969	-0.00814	0.79043	0.00045	10.0 s
35:24.3	Data point 33	1.50000 mL	0.17241 mL	0.14019 mL	0.14000 mL	2.180	-0.00761	0.40848	0.00059	10.0 s
35:59.9	Data point 34	1.50000 mL	0.17241 mL	0.15219 mL	0.14000 mL	2.379	0.01002	0.94066	0.00051	10.0 s
36:35.6	Data point 35	1.50000 mL	0.17241 mL	0.15974 mL	0.14000 mL	2.569	0.00480	0.68312	0.00029	10.0 s
37:11.1	Data point 36	1.50000 mL	0.17241 mL	0.16472 mL	0.14000 mL	2.737	0.00482	0.88092	0.00025	10.0 s

Sample name: **M16_octanol** Experiment start time: **3/1/2018 12:08:09 PM**
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Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01009_M16_octanol_pH-metric high logP.t3r**

Events (continued)

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
38:02.2	Data point 37	1.50000 mL	0.17241 mL	0.16898 mL	0.14000 mL	2.939	-0.00481	0.19222	0.00054	10.0 s
38:53.3	Data point 38	1.50000 mL	0.17241 mL	0.17272 mL	0.14000 mL	3.135	0.00012	0.00403	0.00010	10.0 s
39:39.2	Data point 39	1.50000 mL	0.17241 mL	0.17512 mL	0.14000 mL	3.328	0.00518	0.27140	0.00049	10.0 s
40:25.0	Data point 40	1.50000 mL	0.17241 mL	0.17693 mL	0.14000 mL	3.530	-0.00192	0.46039	0.00014	10.0 s
41:00.4	Data point 41	1.50000 mL	0.17241 mL	0.17858 mL	0.14000 mL	3.764	-0.00045	0.04173	0.00011	10.0 s
41:41.0	Data point 42	1.50000 mL	0.17241 mL	0.17954 mL	0.14000 mL	3.961	0.01048	0.42558	0.00079	10.0 s
42:16.4	Data point 43	1.50000 mL	0.17241 mL	0.18055 mL	0.14000 mL	4.287	0.00274	0.05649	0.00057	10.5 s
42:52.4	Data point 44	1.50000 mL	0.17241 mL	0.18156 mL	0.14000 mL	5.845	-0.01422	0.55499	0.00094	24.0 s
43:47.0	Data point 45	1.50000 mL	0.17241 mL	0.18175 mL	0.14000 mL	6.336	-0.01876	0.92228	0.00096	33.0 s
44:50.5	Data point 46	1.50000 mL	0.17241 mL	0.18184 mL	0.14000 mL	6.906	-0.02960	0.95500	0.00150	Timed out at 59.5 s
46:15.9	Data point 47	1.50000 mL	0.17241 mL	0.18191 mL	0.14000 mL	7.300	-0.02968	0.97977	0.00148	Timed out at 59.5 s
47:46.5	Data point 48	1.50000 mL	0.17241 mL	0.18215 mL	0.14000 mL	8.457	-0.01552	0.97452	0.00078	41.5 s
48:53.6	Data point 49	1.50000 mL	0.17241 mL	0.18248 mL	0.14000 mL	9.131	-0.01766	0.85050	0.00095	15.5 s
49:34.5	Data point 50	1.50000 mL	0.17241 mL	0.18337 mL	0.14000 mL	9.719	-0.00134	0.00466	0.00097	13.0 s
50:13.0	Data point 51	1.50000 mL	0.17241 mL	0.18436 mL	0.14000 mL	10.037	-0.00738	0.26859	0.00070	10.0 s
50:58.7	Data point 52	1.50000 mL	0.17241 mL	0.18532 mL	0.14000 mL	10.233	0.00095	0.02065	0.00033	10.0 s
51:49.7	Data point 53	1.50000 mL	0.17241 mL	0.18667 mL	0.14000 mL	10.421	-0.00379	0.74501	0.00022	10.5 s
52:25.6	Data point 54	1.50000 mL	0.17241 mL	0.18815 mL	0.14000 mL	10.575	-0.00945	0.32573	0.00082	10.0 s
53:16.7	Data point 55	1.50000 mL	0.17241 mL	0.19092 mL	0.14000 mL	10.762	-0.00222	0.36351	0.00018	10.0 s
54:07.8	Data point 56	1.50000 mL	0.17241 mL	0.19405 mL	0.14000 mL	10.955	-0.00583	0.12472	0.00082	10.0 s
54:58.8	Data point 57	1.50000 mL	0.17241 mL	0.19817 mL	0.14000 mL	11.147	-0.00232	0.32508	0.00020	10.0 s
55:44.8	Data point 58	1.50000 mL	0.17241 mL	0.20372 mL	0.14000 mL	11.336	-0.00054	0.03917	0.00013	10.0 s
56:30.8	Data point 59	1.50000 mL	0.17241 mL	0.21129 mL	0.14000 mL	11.529	0.00672	0.53103	0.00046	10.0 s
57:06.5	Data point 60	1.50000 mL	0.17241 mL	0.22204 mL	0.14000 mL	11.710	0.00008	0.00005	0.00057	10.0 s
57:42.4	Data point 61	1.50000 mL	0.17241 mL	0.23838 mL	0.14000 mL	11.894	0.00523	0.08361	0.00089	10.0 s
58:18.3	Data point 62	1.50000 mL	0.17241 mL	0.25654 mL	0.14000 mL	12.032	0.00844	0.20969	0.00091	10.0 s
59:40.6	Data point 63	1.50000 mL	0.31378 mL	0.25654 mL	0.44000 mL	1.970	-0.00419	0.48669	0.00030	10.0 s
1:00:27.0	Data point 64	1.50000 mL	0.31378 mL	0.27848 mL	0.44000 mL	2.183	-0.01035	0.62763	0.00065	20.0 s
1:01:12.7	Data point 65	1.50000 mL	0.31378 mL	0.29229 mL	0.44000 mL	2.381	-0.00423	0.05683	0.00088	10.0 s
1:01:48.4	Data point 66	1.50000 mL	0.31378 mL	0.30115 mL	0.44000 mL	2.559	0.00526	0.10194	0.00081	10.0 s
1:02:24.0	Data point 67	1.50000 mL	0.31378 mL	0.30717 mL	0.44000 mL	2.724	0.00672	0.26884	0.00064	10.0 s
1:03:09.9	Data point 68	1.50000 mL	0.31378 mL	0.31195 mL	0.44000 mL	2.924	0.01126	0.42408	0.00085	18.0 s
1:03:53.4	Data point 69	1.50000 mL	0.31378 mL	0.31512 mL	0.44000 mL	3.103	0.00666	0.70178	0.00039	10.5 s
1:04:29.5	Data point 70	1.50000 mL	0.31378 mL	0.31771 mL	0.44000 mL	3.331	0.00922	0.44168	0.00069	10.5 s
1:05:05.5	Data point 71	1.50000 mL	0.31378 mL	0.32001 mL	0.44000 mL	3.635	0.00860	0.24150	0.00086	10.0 s
1:05:41.0	Data point 72	1.50000 mL	0.31378 mL	0.32117 mL	0.44000 mL	3.886	0.00769	0.25705	0.00075	10.0 s
1:06:16.4	Data point 73	1.50000 mL	0.31378 mL	0.32227 mL	0.44000 mL	4.432	0.00226	0.01769	0.00084	10.5 s
1:06:52.3	Data point 74	1.50000 mL	0.31378 mL	0.32298 mL	0.44000 mL	6.389	-0.01886	0.93280	0.00097	55.5 s
1:08:18.4	Data point 75	1.50000 mL	0.31378 mL	0.32326 mL	0.44000 mL	7.922	-0.05162	0.99435	0.00256	Timed out at 59.5 s
1:09:48.9	Data point 76	1.50000 mL	0.31378 mL	0.32340 mL	0.44000 mL	8.182	-0.01649	0.68209	0.00099	44.0 s
1:10:58.4	Data point 77	1.50000 mL	0.31378 mL	0.32352 mL	0.44000 mL	8.506	-0.01726	0.75067	0.00098	23.0 s
1:11:46.7	Data point 78	1.50000 mL	0.31378 mL	0.32371 mL	0.44000 mL	8.870	-0.01698	0.74469	0.00097	12.0 s
1:12:24.1	Data point 79	1.50000 mL	0.31378 mL	0.32411 mL	0.44000 mL	9.299	-0.01727	0.74481	0.00099	11.0 s
1:13:00.6	Data point 80	1.50000 mL	0.31378 mL	0.32491 mL	0.44000 mL	9.770	-0.01163	0.54195	0.00078	10.0 s
1:13:36.0	Data point 81	1.50000 mL	0.31378 mL	0.32601 mL	0.44000 mL	10.135	-0.00037	0.00108	0.00056	10.0 s
1:14:11.5	Data point 82	1.50000 mL	0.31378 mL	0.32709 mL	0.44000 mL	10.357	-0.00019	0.00290	0.00018	10.0 s
1:14:57.2	Data point 83	1.50000 mL	0.31378 mL	0.32858 mL	0.44000 mL	10.542	0.00649	0.22886	0.00067	10.0 s
1:15:48.3	Data point 84	1.50000 mL	0.31378 mL	0.33088 mL	0.44000 mL	10.732	0.00792	0.45250	0.00058	10.0 s
1:16:23.8	Data point 85	1.50000 mL	0.31378 mL	0.33349 mL	0.44000 mL	10.912	0.00857	0.47694	0.00061	10.0 s
1:16:59.3	Data point 86	1.50000 mL	0.31378 mL	0.33688 mL	0.44000 mL	11.093	0.00726	0.16909	0.00087	10.0 s
1:17:34.9	Data point 87	1.50000 mL	0.31378 mL	0.34163 mL	0.44000 mL	11.245	0.00646	0.13436	0.00087	10.0 s
1:18:26.0	Data point 88	1.50000 mL	0.31378 mL	0.34962 mL	0.44000 mL	11.440	0.00609	0.16576	0.00074	10.0 s
1:19:12.1	Data point 89	1.50000 mL	0.31378 mL	0.36091 mL	0.44000 mL	11.639	0.01231	0.61053	0.00078	22.5 s
1:20:00.5	Data point 90	1.50000 mL	0.31378 mL	0.37676 mL	0.44000 mL	11.816	0.00711	0.92311	0.00037	10.0 s

Sample name: **M16_octanol** Experiment start time: **3/1/2018 12:08:09 PM**
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Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01009_M16_octanol_pH-metric high logP.t3r**

Events (continued)

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
1:20:36.5	Data point 91	1.50000 mL	0.31378 mL	0.40127 mL	0.44000 mL	11.997	0.01097	0.61510	0.00069	10.0 s
1:21:12.1	Data point 92	1.50000 mL	0.31378 mL	0.40837 mL	0.44000 mL	12.034	0.01274	0.67396	0.00077	10.0 s
1:21:31.3	Assay volumes	1.50000 mL	0.31378 mL	0.40837 mL	0.44000 mL					

Sample name: **M16_octanol** Experiment start time: **3/1/2018 12:08:09 PM**
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Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01009_M16_octanol_pH-metric high logP.t3r**

Assay Settings

Setting	Value	Original Value	Date/Time changed	Imported from
General Settings				
Analyst name	Pion			
Standard Experiment Settings				
Number of titrations	3			
Minimum pH	2.000			
Maximum pH	12.000			
pH step between points of	0.200			
Minimum titrant addition	0.00002 mL			
Maximum titrant addition	0.10000 mL			
Argon flow rate	100%			
Start titration using	Cautious pH adjust			
Advanced General Settings				
Detect turbidity using	None			
Collect turbidity sensor data	No			
Collect UV spectra	No			
Stir after titrant addition for	5 seconds			
For titrant addition, stir at	10%			
Titrant Pre-Dose				
Titrant pre-dose	None			
Assay Medium				
ISA water volume	1.50 mL			
Water added	Automatic			
Partition solvent type	Octanol			
Partition volume	0.040 mL			
Partition solvent added	Automatic			
After partition addition, stir for	1 seconds			
Sample Sonication				
Sonicate	Yes			
Adjust pH for sonication	No			
Sonicate for	300 seconds			
After sonication stir for	5 seconds			
Sample Dissolution				
Perform a dissolution stage	Yes			
Adjust and hold pH for dissolution	To start pH			
Stir to dissolve for	120 seconds			
For dissolution, stir at	10%			
Carbonate purge				
Perform a carbonate purge	No			
Temperature Control				
Wait for temperature	Yes			
Required start temperature	25.0°C			
Acceptable deviation	0.5°C			
Time to wait	60 seconds			
Stir speed of	50%			
Titration 1				
Titrate from	Low to high pH			
Adjust to start pH	Yes			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	50%			
Titration 2				
Titrate from	Low to high pH			
Add additional water	0.00 mL			
Additional partition solvent volume	0.100 mL			
Additional partition solvent added	Automatic			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	55%			

Sample name: **M16_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01009**
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Experiment start time: **3/1/2018 12:08:09 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
Titration 3				
Titrate from	Low to high pH			
Add additional water	0.00 mL			
Additional partition solvent volume	0.300 mL			
Additional partition solvent added	Automatic			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	60%			
Data Point Stability				
Stir during data point collection	No			
Delay before data point collection	0 seconds			
Number of points to average	20 points			
Time interval between points	0.50 seconds			
Required maximum standard deviation	0.00100 dpH/dt			
Stability timeout after	60 seconds			

Calibration Settings

Setting	Value	Date/Time changed	Imported from
Four-Plus alpha	0.130	3/1/2018 12:08:08 PM	C:\Sirius_T3\HCl18B27.t3r
Four-Plus S	0.9970	3/1/2018 12:08:08 PM	C:\Sirius_T3\HCl18B27.t3r
Four-Plus jH	0.8	3/1/2018 12:08:08 PM	C:\Sirius_T3\HCl18B27.t3r
Four-Plus jOH	-0.4	3/1/2018 12:08:08 PM	C:\Sirius_T3\HCl18B27.t3r
Base concentration factor	1.000	3/1/2018 12:08:09 PM	C:\Sirius_T3\KOH18B27.t3r
Acid concentration factor	0.994	3/1/2018 12:08:08 PM	C:\Sirius_T3\HCl18B27.t3r

Instrument Settings

Setting	Value	Batch Id	Install date
Instrument owner	Merck		
Instrument ID	T312060		
Instrument type	T3 Simulator		
Software version	1.1.3.0		
Dispenser module		T3DM1200361	3/31/2009 5:24:52 AM
Dispenser 0	Water		3/31/2009 5:25:05 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Water (0.15 M KCl)	02-06-2018	2/27/2018 10:05:59 AM
Dispenser 2	Acid		3/31/2009 5:25:11 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Acid (0.5 M HCl)	02-27-2018	2/27/2018 10:27:22 AM
Dispenser 1	Base		3/31/2009 5:25:21 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Base (0.5 M KOH)	9/22/2017	2/27/2018 10:21:22 AM
Dispenser 5	Cosolvent		3/31/2009 5:26:24 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Distribution valve 5	Distribution Valve		3/31/2009 5:28:19 AM
Firmware version	1.1.3		
Port A	Methanol (80%, 0.15 M KCl)	09-26-17	2/7/2018 9:42:01 AM
Port B	Cyclohexane	11-01-17	2/27/2018 10:37:57 AM
Dispenser 3	Buffer		8/3/2010 5:05:16 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Dodecane	2018/01/31	2/28/2018 10:18:04 AM
Dispenser 6	Octanol		10/22/2010 10:52:43 AM

Sample name: **M16_octanol**   Experiment start time: **3/1/2018 12:08:09 PM**
Assay name: **pH-metric high logP**   Analyst: **Pion**
Assay ID: **18C-01009**   Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01009_M16_octanol_pH-metric high logP.t3r**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Octanol	01-31-2018	2/27/2018 9:59:35 AM
Titrator		T3TM1200161	3/31/2009 5:24:17 AM
Horizontal axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Probe I/O firmware version	1.1.1		
Electrode	T3 Electrode	T3E0923	1/23/2018 2:01:00 PM
E0 calibration	+4.26 mV		3/1/2018 12:08:36 PM
Filling solution	3M KCl	KCL097	2/27/2018 9:49:43 AM
Liquids			
Wash 1	50% IPA:50% Water		2/28/2018 10:23:32 AM
Wash 2	0.5% Trition X-100 in H20		2/28/2018 10:23:34 AM
Buffer position 1	pH7 Wash		2/28/2018 10:24:06 AM
Buffer position 2	pH 7		2/28/2018 10:24:08 AM
Storage position			2/28/2018 10:21:14 AM
Wash water	8.2e+003 mL	02-27-2018	2/27/2018 9:54:39 AM
Waste	7.3e+003 mL		11/28/2017 10:36:29 AM
Temperature controller			8/5/2010 6:35:13 AM
Turbidity detector			3/31/2009 5:24:45 AM
Spectrometer		074811	11/23/2010 11:22:28 AM
Dip probe		10196	
Wavelength coefficient A0	183.333		
Wavelength coefficient A1	2.21568		
Wavelength coefficient A2	-0.000289308		
Total lamp lit time	112:08:55		11/23/2010 11:22:28 AM
Calibrated on	2/27/2018 10:40:38 AM		
Integration time	40		
Scans averaged	10		
Autoloader		T3AL1200345	11/10/2015 9:34:13 AM
Left-right axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Front-back axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Configuration			
Alternate titration position	Titration position		
Alternate reference position	Reference position		
Maximum standard vial volume	3.50 mL		
Maximum alternate vial volume	25.00 mL		
Automatic action idle period	5 minute(s)		
Titrant tube volume	1.3 mL		
Syringe flush count	3.50		
Flowing wash pump volume	20.0 mL		
Flowing wash stir duration	5 s		
Flowing wash stir speed	30%		
Solvent wash stir duration	5 s		
Solvent wash stir speed	30%		
Surfactant wash stir duration	5 s		
Surfactant wash stir speed	30%		
E0 calibration minimum number of points	10		
E0 calibration maximum standard deviation	0.01500		
E0 calibration timeout period	60 s		
E0 calibration stir duration	5 s		
E0 calibration preparation stir speed	30%		
E0 calibration buffer wash stir duration	5 s		
E0 calibration buffer wash stir speed	30%		
E0 calibration reading stir speed	0%		

Sample name: **M16_octanol**

Assay name: **pH-metric high logP**

Assay ID: **18C-01009**

Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01009_M16_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 12:08:09 PM**

Analyst: **Pion**

Instrument ID: **T312060**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Spectrometer calibration stir duration	5 s		
Spectrometer calibration stir speed	30%		
Spectrometer calibration wash pump volume	20.0 mL		
Spectrometer calibration wash stir duration	5 s		
Spectrometer calibration wash stir speed	30%		
Overhead dispense height	10000		

Refinement Settings

Setting	Value	Default value
Turbidity detection method	None	None
Turbidity wavelength to assess	500.0 nm	500.0 nm
Turbidity maximum absorbance	0.100	0.100
Turbidity probe threshold	50.00	50.00

Experiment Log

[2:16] Air gap created for Water (0.15 M KCl)
[2:17] Air gap created for Acid (0.5 M HCl)
[2:17] Air gap created for Base (0.5 M KOH)
[2:17] Air gap released for Water (0.15 M KCl)
[2:21] Titrator arm moved over Titration position
[2:21] Titration 1 of 3
[2:21] Adding initial titrants
[2:21] Automatically add 1.50000 mL of water
[2:46] Dispensed 1.500000 mL of Water (0.15 M KCl)
[2:51] Titrator arm moved over Drain
[8:32] Titrator arm moved to Titration position
[8:32] Argon flow rate set to 100
[8:32] Stirrer speed set to 10
[8:37] Automatically add 0.04000 mL of Octanol
[8:38] Dispensed 0.040005 mL of Octanol
[8:39] Initial pH = 3.74
[8:39] Iterative adjust 3.74 -> 2.00
[8:39] pH 3.74 -> 2.00
[8:41] Air gap released for Acid (0.5 M HCl)
[8:41] Dispensed 0.042615 mL of Acid (0.5 M HCl)
[8:46] pH 2.02 -> 2.00
[8:47] Dispensed 0.002375 mL of Acid (0.5 M HCl)
[8:52] Holding pH 2.00
[10:52] Stirrer speed set to 0
[10:52] Stirrer speed set to 50
[10:52] Iterative adjust 1.98 -> 2.00
[10:52] pH 1.98 -> 2.00
[10:53] Air gap released for Base (0.5 M KOH)
[10:53] Dispensed 0.002023 mL of Base (0.5 M KOH)
[11:44] Stirrer speed set to 0
[11:54] Datapoint id 1 collected
[11:54] Stirrer speed set to 50
[11:59] pH 2.02 -> 2.22
[11:59] Using cautious pH adjust
[11:59] Dispensed 0.007596 mL of Base (0.5 M KOH)
[12:04] Stepping pH = 2.10
[12:04] Dispensed 0.005997 mL of Base (0.5 M KOH)
[12:10] Stepping pH = 2.19
[12:10] Dispensed 0.001646 mL of Base (0.5 M KOH)
[12:15] Stepping pH = 2.22
[12:30] Stirrer speed set to 0
[12:40] Datapoint id 2 collected

Sample name: **M16_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01009**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01009_M16_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 12:08:09 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[12:40] Charge balance equation is out by -0.2%
[12:40] Stirrer speed set to 50
[12:45] pH 2.23 -> 2.43
[12:45] Using charge balance adjust
[12:45] Dispensed 0.009407 mL of Base (0.5 M KOH)
[13:06] Stirrer speed set to 0
[13:16] Datapoint id 3 collected
[13:16] Charge balance equation is out by -6.0%
[13:16] Stirrer speed set to 50
[13:21] pH 2.42 -> 2.62
[13:21] Using charge balance adjust
[13:21] Dispensed 0.006021 mL of Base (0.5 M KOH)
[13:41] Stirrer speed set to 0
[13:51] Datapoint id 4 collected
[13:51] Charge balance equation is out by -18.1%
[13:51] Stirrer speed set to 50
[13:56] pH 2.59 -> 2.79
[13:56] Using cautious pH adjust
[13:56] Dispensed 0.002046 mL of Base (0.5 M KOH)
[14:01] Stepping pH = 2.67
[14:02] Dispensed 0.001787 mL of Base (0.5 M KOH)
[14:07] Stepping pH = 2.76
[14:07] Dispensed 0.000494 mL of Base (0.5 M KOH)
[14:12] Stepping pH = 2.78
[14:27] Stirrer speed set to 0
[14:37] Datapoint id 5 collected
[14:37] Charge balance equation is out by -5.4%
[14:37] Stirrer speed set to 50
[14:42] pH 2.79 -> 2.99
[14:42] Using charge balance adjust
[14:42] Dispensed 0.002705 mL of Base (0.5 M KOH)
[15:02] Stirrer speed set to 0
[15:12] Datapoint id 6 collected
[15:12] Charge balance equation is out by -31.5%
[15:12] Stirrer speed set to 50
[15:18] pH 2.93 -> 3.13
[15:18] Using cautious pH adjust
[15:18] Dispensed 0.001035 mL of Base (0.5 M KOH)
[15:23] Stepping pH = 2.99
[15:23] Dispensed 0.001294 mL of Base (0.5 M KOH)
[15:28] Stepping pH = 3.08
[15:28] Dispensed 0.000541 mL of Base (0.5 M KOH)
[15:33] Stepping pH = 3.12
[15:48] Stirrer speed set to 0
[15:58] Datapoint id 7 collected
[15:58] Charge balance equation is out by -39.0%
[15:58] Stirrer speed set to 50
[16:03] pH 3.12 -> 3.32
[16:03] Using cautious pH adjust
[16:04] Dispensed 0.000753 mL of Base (0.5 M KOH)
[16:09] Stepping pH = 3.18
[16:09] Dispensed 0.000917 mL of Base (0.5 M KOH)
[16:14] Stepping pH = 3.27
[16:14] Dispensed 0.000423 mL of Base (0.5 M KOH)
[16:19] Stepping pH = 3.30
[16:19] Dispensed 0.000165 mL of Base (0.5 M KOH)
[16:24] Stepping pH = 3.32
[16:39] Stirrer speed set to 0
[16:49] Datapoint id 8 collected

Sample name: **M16_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01009**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01009_M16_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 12:08:09 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[16:49] Charge balance equation is out by -50.3%
[16:49] Stirrer speed set to 50
[16:55] pH 3.32 -> 3.52
[16:55] Using cautious pH adjust
[16:55] Dispensed 0.000611 mL of Base (0.5 M KOH)
[17:00] Stepping pH = 3.37
[17:00] Dispensed 0.000823 mL of Base (0.5 M KOH)
[17:05] Stepping pH = 3.45
[17:05] Dispensed 0.000541 mL of Base (0.5 M KOH)
[17:10] Stepping pH = 3.49
[17:10] Dispensed 0.000235 mL of Base (0.5 M KOH)
[17:15] Stepping pH = 3.51
[17:30] Stirrer speed set to 0
[17:40] Datapoint id 9 collected
[17:40] Charge balance equation is out by -79.1%
[17:40] Stirrer speed set to 50
[17:45] pH 3.51 -> 3.71
[17:45] Using cautious pH adjust
[17:46] Dispensed 0.000588 mL of Base (0.5 M KOH)
[17:51] Stepping pH = 3.56
[17:51] Dispensed 0.000800 mL of Base (0.5 M KOH)
[17:56] Stepping pH = 3.63
[17:56] Dispensed 0.000635 mL of Base (0.5 M KOH)
[18:01] Stepping pH = 3.69
[18:01] Dispensed 0.000118 mL of Base (0.5 M KOH)
[18:06] Stepping pH = 3.70
[18:21] Stirrer speed set to 0
[18:31] Datapoint id 10 collected
[18:31] Charge balance equation is out by -81.1%
[18:31] Stirrer speed set to 50
[18:37] pH 3.70 -> 3.90
[18:37] Using cautious pH adjust
[18:37] Dispensed 0.000635 mL of Base (0.5 M KOH)
[18:42] Stepping pH = 3.77
[18:42] Dispensed 0.000729 mL of Base (0.5 M KOH)
[18:47] Stepping pH = 3.86
[18:47] Dispensed 0.000259 mL of Base (0.5 M KOH)
[18:52] Stepping pH = 3.89
[18:52] Dispensed 0.000094 mL of Base (0.5 M KOH)
[18:57] Stepping pH = 3.89
[19:12] Stirrer speed set to 0
[19:22] Datapoint id 11 collected
[19:22] Charge balance equation is out by -36.1%
[19:22] Stirrer speed set to 50
[19:27] pH 3.89 -> 4.09
[19:27] Using cautious pH adjust
[19:28] Dispensed 0.000753 mL of Base (0.5 M KOH)
[19:33] Stepping pH = 4.04
[19:33] Dispensed 0.000282 mL of Base (0.5 M KOH)
[19:38] Stepping pH = 4.08
[19:38] Dispensed 0.000071 mL of Base (0.5 M KOH)
[19:43] Stepping pH = 4.08
[19:43] Dispensed 0.000141 mL of Base (0.5 M KOH)
[19:48] Stepping pH = 4.11
[20:03] Stirrer speed set to 0
[20:13] Datapoint id 12 collected
[20:13] Charge balance equation is out by 17.6%
[20:13] Stirrer speed set to 50
[20:18] pH 4.11 -> 4.31

Sample name: **M16_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01009**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01009_M16_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 12:08:09 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[20:18] Using cautious pH adjust
[20:18] Dispensed 0.000894 mL of Base (0.5 M KOH)
[20:24] Stepping pH = 4.40
[20:39] Stirrer speed set to 0
[20:49] Datapoint id 13 collected
[20:49] Charge balance equation is out by 50.0%
[20:49] Stirrer speed set to 50
[20:54] pH 4.39 -> 4.59
[20:54] Using cautious pH adjust
[20:54] Dispensed 0.001011 mL of Base (0.5 M KOH)
[21:00] Stepping pH = 5.11
[21:15] Stirrer speed set to 0
[21:28] Datapoint id 14 collected
[21:28] Charge balance equation is out by 50.0%
[21:28] Stirrer speed set to 50
[21:33] pH 5.12 -> 5.32
[21:33] Using cautious pH adjust
[21:33] Dispensed 0.000611 mL of Base (0.5 M KOH)
[21:38] Stepping pH = 8.25
[21:53] Stirrer speed set to 0
[22:28] Datapoint id 15 collected
[22:28] Charge balance equation is out by 50.0%
[22:28] Stirrer speed set to 50
[22:33] pH 8.53 -> 8.73
[22:33] Using cautious pH adjust
[22:33] Dispensed 0.000588 mL of Base (0.5 M KOH)
[22:38] Stepping pH = 9.19
[22:53] Stirrer speed set to 0
[23:03] Datapoint id 16 collected
[23:03] Charge balance equation is out by 50.0%
[23:03] Stirrer speed set to 50
[23:08] pH 9.18 -> 9.38
[23:08] Using cautious pH adjust
[23:08] Dispensed 0.001011 mL of Base (0.5 M KOH)
[23:13] Stepping pH = 9.60
[23:28] Stirrer speed set to 0
[23:38] Datapoint id 17 collected
[23:38] Charge balance equation is out by 50.0%
[23:38] Stirrer speed set to 50
[23:44] pH 9.59 -> 9.79
[23:44] Using cautious pH adjust
[23:44] Dispensed 0.000847 mL of Base (0.5 M KOH)
[23:49] Stepping pH = 9.79
[24:04] Stirrer speed set to 0
[24:14] Datapoint id 18 collected
[24:14] Charge balance equation is out by 50.0%
[24:14] Stirrer speed set to 50
[24:19] pH 9.78 -> 9.98
[24:19] Using cautious pH adjust
[24:19] Dispensed 0.000729 mL of Base (0.5 M KOH)
[24:24] Stepping pH = 9.91
[24:24] Dispensed 0.000282 mL of Base (0.5 M KOH)
[24:29] Stepping pH = 9.94
[24:30] Dispensed 0.000282 mL of Base (0.5 M KOH)
[24:35] Stepping pH = 9.98
[24:50] Stirrer speed set to 0
[25:00] Datapoint id 19 collected
[25:00] Charge balance equation is out by 10.9%
[25:00] Stirrer speed set to 50

Sample name: **M16_octanol**   Experiment start time: **3/1/2018 12:08:09 PM**
Assay name: **pH-metric high logP**   Analyst: **Pion**
Assay ID: **18C-01009**   Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01009_M16_octanol_pH-metric high logP.t3r**

Experiment Log (continued)

[25:05] pH 9.98 -> 10.18
[25:05] Using charge balance adjust
[25:05] Dispensed 0.001199 mL of Base (0.5 M KOH)
[25:26] Stirrer speed set to 0
[25:36] Datapoint id 20 collected
[25:36] Charge balance equation is out by -11.3%
[25:36] Stirrer speed set to 50
[25:41] pH 10.16 -> 10.36
[25:41] Using charge balance adjust
[25:41] Dispensed 0.001082 mL of Base (0.5 M KOH)
[26:01] Stirrer speed set to 0
[26:11] Datapoint id 21 collected
[26:11] Charge balance equation is out by -32.3%
[26:11] Stirrer speed set to 50
[26:16] pH 10.29 -> 10.49
[26:16] Using cautious pH adjust
[26:16] Dispensed 0.000517 mL of Base (0.5 M KOH)
[26:21] Stepping pH = 10.36
[26:21] Dispensed 0.000611 mL of Base (0.5 M KOH)
[26:27] Stepping pH = 10.43
[26:27] Dispensed 0.000353 mL of Base (0.5 M KOH)
[26:32] Stepping pH = 10.47
[26:32] Dispensed 0.000165 mL of Base (0.5 M KOH)
[26:37] Stepping pH = 10.49
[26:52] Stirrer speed set to 0
[27:02] Datapoint id 22 collected
[27:02] Charge balance equation is out by -58.4%
[27:02] Stirrer speed set to 50
[27:07] pH 10.48 -> 10.68
[27:07] Using cautious pH adjust
[27:07] Dispensed 0.000588 mL of Base (0.5 M KOH)
[27:12] Stepping pH = 10.55
[27:12] Dispensed 0.000682 mL of Base (0.5 M KOH)
[27:18] Stepping pH = 10.61
[27:18] Dispensed 0.000494 mL of Base (0.5 M KOH)
[27:23] Stepping pH = 10.66
[27:23] Dispensed 0.000188 mL of Base (0.5 M KOH)
[27:28] Stepping pH = 10.68
[27:43] Stirrer speed set to 0
[27:53] Datapoint id 23 collected
[27:53] Charge balance equation is out by -67.1%
[27:53] Stirrer speed set to 50
[27:58] pH 10.67 -> 10.87
[27:58] Using cautious pH adjust
[27:58] Dispensed 0.000729 mL of Base (0.5 M KOH)
[28:03] Stepping pH = 10.73
[28:03] Dispensed 0.000964 mL of Base (0.5 M KOH)
[28:08] Stepping pH = 10.80
[28:09] Dispensed 0.000706 mL of Base (0.5 M KOH)
[28:14] Stepping pH = 10.84
[28:14] Dispensed 0.000306 mL of Base (0.5 M KOH)
[28:19] Stepping pH = 10.86
[28:34] Stirrer speed set to 0
[28:45] Datapoint id 24 collected
[28:45] Charge balance equation is out by -85.3%
[28:45] Stirrer speed set to 50
[28:50] pH 10.85 -> 11.05
[28:50] Using cautious pH adjust
[28:50] Dispensed 0.001011 mL of Base (0.5 M KOH)

Sample name: **M16_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01009**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01009_M16_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 12:08:09 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[28:55] Stepping pH = 10.91
[28:55] Dispensed 0.001270 mL of Base (0.5 M KOH)
[29:00] Stepping pH = 11.00
[29:00] Dispensed 0.000682 mL of Base (0.5 M KOH)
[29:05] Stepping pH = 11.04
[29:05] Dispensed 0.000165 mL of Base (0.5 M KOH)
[29:11] Stepping pH = 11.05
[29:26] Stirrer speed set to 0
[29:36] Datapoint id 25 collected
[29:36] Charge balance equation is out by -55.8%
[29:36] Stirrer speed set to 50
[29:41] pH 11.04 -> 11.24
[29:41] Using cautious pH adjust
[29:41] Dispensed 0.001505 mL of Base (0.5 M KOH)
[29:46] Stepping pH = 11.13
[29:46] Dispensed 0.001364 mL of Base (0.5 M KOH)
[29:51] Stepping pH = 11.21
[29:51] Dispensed 0.000541 mL of Base (0.5 M KOH)
[29:56] Stepping pH = 11.23
[30:11] Stirrer speed set to 0
[30:22] Datapoint id 26 collected
[30:22] Charge balance equation is out by -13.7%
[30:22] Stirrer speed set to 50
[30:27] pH 11.23 -> 11.43
[30:27] Using charge balance adjust
[30:27] Dispensed 0.004516 mL of Base (0.5 M KOH)
[30:47] Stirrer speed set to 0
[30:57] Datapoint id 27 collected
[30:57] Charge balance equation is out by -16.5%
[30:57] Stirrer speed set to 50
[31:02] pH 11.40 -> 11.60
[31:02] Using cautious pH adjust
[31:02] Dispensed 0.003340 mL of Base (0.5 M KOH)
[31:07] Stepping pH = 11.51
[31:08] Dispensed 0.002187 mL of Base (0.5 M KOH)
[31:13] Stepping pH = 11.57
[31:13] Dispensed 0.000847 mL of Base (0.5 M KOH)
[31:18] Stepping pH = 11.59
[31:33] Stirrer speed set to 0
[31:43] Datapoint id 28 collected
[31:43] Charge balance equation is out by 4.5%
[31:43] Stirrer speed set to 50
[31:48] pH 11.59 -> 11.79
[31:48] Using charge balance adjust
[31:48] Dispensed 0.010583 mL of Base (0.5 M KOH)
[32:09] Stirrer speed set to 0
[32:19] Datapoint id 29 collected
[32:19] Charge balance equation is out by -12.6%
[32:19] Stirrer speed set to 50
[32:24] pH 11.77 -> 11.97
[32:24] Using charge balance adjust
[32:24] Dispensed 0.016157 mL of Base (0.5 M KOH)
[32:44] Stirrer speed set to 0
[32:55] Datapoint id 30 collected
[32:55] Charge balance equation is out by -7.8%
[32:55] Stirrer speed set to 50
[33:00] pH 11.96 -> 12.05
[33:00] Using charge balance adjust
[33:00] Dispensed 0.009737 mL of Base (0.5 M KOH)

Sample name: **M16_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01009**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01009_M16_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 12:08:09 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[33:20] Stirrer speed set to 0
[33:30] Datapoint id 31 collected
[33:30] Charge balance equation is out by -63.2%
[33:30] Titration 2 of 3
[33:30] Adding initial titrants
[33:30] Automatically add 0.10000 mL of Octanol
[33:33] Dispensed 0.100000 mL of Octanol
[33:33] Stirrer speed set to 10
[33:34] Stirrer speed set to 55
[33:34] Iterative adjust 12.04 -> 2.00
[33:34] pH 12.04 -> 2.00
[33:36] Dispensed 0.100000 mL of Acid (0.5 M HCl)
[33:41] pH 2.31 -> 2.00
[33:42] Dispensed 0.025141 mL of Acid (0.5 M HCl)
[33:47] pH 2.02 -> 2.00
[33:47] Dispensed 0.002281 mL of Acid (0.5 M HCl)
[34:38] Stirrer speed set to 0
[34:48] Datapoint id 32 collected
[34:48] Stirrer speed set to 55
[34:53] pH 1.98 -> 2.18
[34:53] Using cautious pH adjust
[34:53] Dispensed 0.009784 mL of Base (0.5 M KOH)
[34:58] Stepping pH = 2.06
[34:58] Dispensed 0.007502 mL of Base (0.5 M KOH)
[35:03] Stepping pH = 2.15
[35:04] Dispensed 0.001999 mL of Base (0.5 M KOH)
[35:09] Stepping pH = 2.18
[35:24] Stirrer speed set to 0
[35:34] Datapoint id 33 collected
[35:34] Charge balance equation is out by 1.4%
[35:34] Stirrer speed set to 55
[35:39] pH 2.19 -> 2.39
[35:39] Using charge balance adjust
[35:39] Dispensed 0.011994 mL of Base (0.5 M KOH)
[35:59] Stirrer speed set to 0
[36:10] Datapoint id 34 collected
[36:10] Charge balance equation is out by -3.2%
[36:10] Stirrer speed set to 55
[36:15] pH 2.39 -> 2.59
[36:15] Using charge balance adjust
[36:15] Dispensed 0.007549 mL of Base (0.5 M KOH)
[36:35] Stirrer speed set to 0
[36:45] Datapoint id 35 collected
[36:45] Charge balance equation is out by -9.6%
[36:45] Stirrer speed set to 55
[36:50] pH 2.58 -> 2.78
[36:50] Using charge balance adjust
[36:50] Dispensed 0.004986 mL of Base (0.5 M KOH)
[37:11] Stirrer speed set to 0
[37:21] Datapoint id 36 collected
[37:21] Charge balance equation is out by -20.0%
[37:21] Stirrer speed set to 55
[37:26] pH 2.74 -> 2.94
[37:26] Using cautious pH adjust
[37:26] Dispensed 0.001764 mL of Base (0.5 M KOH)
[37:31] Stepping pH = 2.82
[37:31] Dispensed 0.001623 mL of Base (0.5 M KOH)
[37:36] Stepping pH = 2.90
[37:36] Dispensed 0.000659 mL of Base (0.5 M KOH)

Sample name: **M16_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01009**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01009_M16_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 12:08:09 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[37:41] Stepping pH = 2.93
[37:42] Dispensed 0.000212 mL of Base (0.5 M KOH)
[37:47] Stepping pH = 2.94
[38:02] Stirrer speed set to 0
[38:12] Datapoint id 37 collected
[38:12] Charge balance equation is out by -20.5%
[38:12] Stirrer speed set to 55
[38:17] pH 2.94 -> 3.14
[38:17] Using cautious pH adjust
[38:17] Dispensed 0.001223 mL of Base (0.5 M KOH)
[38:22] Stepping pH = 3.00
[38:22] Dispensed 0.001529 mL of Base (0.5 M KOH)
[38:27] Stepping pH = 3.08
[38:27] Dispensed 0.000823 mL of Base (0.5 M KOH)
[38:33] Stepping pH = 3.13
[38:33] Dispensed 0.000165 mL of Base (0.5 M KOH)
[38:38] Stepping pH = 3.14
[38:53] Stirrer speed set to 0
[39:03] Datapoint id 38 collected
[39:03] Charge balance equation is out by -53.0%
[39:03] Stirrer speed set to 55
[39:08] pH 3.14 -> 3.34
[39:08] Using cautious pH adjust
[39:08] Dispensed 0.000941 mL of Base (0.5 M KOH)
[39:13] Stepping pH = 3.21
[39:13] Dispensed 0.001035 mL of Base (0.5 M KOH)
[39:18] Stepping pH = 3.30
[39:18] Dispensed 0.000423 mL of Base (0.5 M KOH)
[39:24] Stepping pH = 3.33
[39:39] Stirrer speed set to 0
[39:49] Datapoint id 39 collected
[39:49] Charge balance equation is out by -27.4%
[39:49] Stirrer speed set to 55
[39:54] pH 3.34 -> 3.54
[39:54] Using cautious pH adjust
[39:54] Dispensed 0.000823 mL of Base (0.5 M KOH)
[39:59] Stepping pH = 3.42
[39:59] Dispensed 0.000753 mL of Base (0.5 M KOH)
[40:04] Stepping pH = 3.51
[40:04] Dispensed 0.000235 mL of Base (0.5 M KOH)
[40:09] Stepping pH = 3.53
[40:25] Stirrer speed set to 0
[40:35] Datapoint id 40 collected
[40:35] Charge balance equation is out by -8.9%
[40:35] Stirrer speed set to 55
[40:40] pH 3.53 -> 3.73
[40:40] Using charge balance adjust
[40:40] Dispensed 0.001646 mL of Base (0.5 M KOH)
[41:00] Stirrer speed set to 0
[41:10] Datapoint id 41 collected
[41:10] Charge balance equation is out by 16.2%
[41:10] Stirrer speed set to 55
[41:15] pH 3.77 -> 3.97
[41:15] Using cautious pH adjust
[41:15] Dispensed 0.000917 mL of Base (0.5 M KOH)
[41:20] Stepping pH = 3.96
[41:20] Dispensed 0.000047 mL of Base (0.5 M KOH)
[41:25] Stepping pH = 3.96
[41:41] Stirrer speed set to 0

Sample name: **M16_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01009**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01009_M16_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 12:08:09 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[41:51] Datapoint id 42 collected
[41:51] Charge balance equation is out by 47.0%
[41:51] Stirrer speed set to 55
[41:56] pH 3.97 -> 4.17
[41:56] Using cautious pH adjust
[41:56] Dispensed 0.001011 mL of Base (0.5 M KOH)
[42:01] Stepping pH = 4.29
[42:16] Stirrer speed set to 0
[42:27] Datapoint id 43 collected
[42:27] Charge balance equation is out by 50.0%
[42:27] Stirrer speed set to 55
[42:32] pH 4.29 -> 4.49
[42:32] Using cautious pH adjust
[42:32] Dispensed 0.001011 mL of Base (0.5 M KOH)
[42:37] Stepping pH = 5.79
[42:52] Stirrer speed set to 0
[43:16] Datapoint id 44 collected
[43:16] Charge balance equation is out by 50.0%
[43:16] Stirrer speed set to 55
[43:21] pH 5.84 -> 6.04
[43:21] Using cautious pH adjust
[43:21] Dispensed 0.000118 mL of Base (0.5 M KOH)
[43:26] Stepping pH = 5.94
[43:26] Dispensed 0.000071 mL of Base (0.5 M KOH)
[43:31] Stepping pH = 6.18
[43:46] Stirrer speed set to 0
[44:20] Datapoint id 45 collected
[44:20] Charge balance equation is out by 18.2%
[44:20] Stirrer speed set to 55
[44:25] pH 6.29 -> 6.49
[44:25] Using cautious pH adjust
[44:25] Dispensed 0.000047 mL of Base (0.5 M KOH)
[44:30] Stepping pH = 6.38
[44:30] Dispensed 0.000047 mL of Base (0.5 M KOH)
[44:35] Stepping pH = 6.89
[44:50] Stirrer speed set to 0
[45:50] Datapoint id 46 collected
[45:50] Charge balance equation is out by 7.4%
[45:50] Stirrer speed set to 55
[45:55] pH 6.83 -> 7.03
[45:55] Using charge balance adjust
[45:55] Dispensed 0.000071 mL of Base (0.5 M KOH)
[46:15] Stirrer speed set to 0
[47:15] Datapoint id 47 collected
[47:15] Charge balance equation is out by 136.7%
[47:15] Stirrer speed set to 55
[47:21] pH 7.23 -> 7.43
[47:21] Using cautious pH adjust
[47:21] Dispensed 0.000024 mL of Base (0.5 M KOH)
[47:26] Stepping pH = 7.19
[47:26] Dispensed 0.000212 mL of Base (0.5 M KOH)
[47:31] Stepping pH = 8.55
[47:46] Stirrer speed set to 0
[48:28] Datapoint id 48 collected
[48:28] Charge balance equation is out by -241.0%
[48:28] Stirrer speed set to 55
[48:33] pH 8.44 -> 8.64
[48:33] Using cautious pH adjust
[48:33] Dispensed 0.000329 mL of Base (0.5 M KOH)

Sample name: **M16_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01009**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01009_M16_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 12:08:09 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[48:38] Stepping pH = 9.15
[48:53] Stirrer speed set to 0
[49:09] Datapoint id 49 collected
[49:09] Charge balance equation is out by 50.0%
[49:09] Stirrer speed set to 55
[49:14] pH 9.13 -> 9.33
[49:14] Using cautious pH adjust
[49:14] Dispensed 0.000894 mL of Base (0.5 M KOH)
[49:19] Stepping pH = 9.72
[49:34] Stirrer speed set to 0
[49:47] Datapoint id 50 collected
[49:47] Charge balance equation is out by 50.0%
[49:47] Stirrer speed set to 55
[49:52] pH 9.72 -> 9.92
[49:52] Using cautious pH adjust
[49:52] Dispensed 0.000988 mL of Base (0.5 M KOH)
[49:57] Stepping pH = 10.04
[50:12] Stirrer speed set to 0
[50:23] Datapoint id 51 collected
[50:23] Charge balance equation is out by 50.0%
[50:23] Stirrer speed set to 55
[50:28] pH 10.04 -> 10.24
[50:28] Using cautious pH adjust
[50:28] Dispensed 0.000800 mL of Base (0.5 M KOH)
[50:33] Stepping pH = 10.22
[50:33] Dispensed 0.000071 mL of Base (0.5 M KOH)
[50:38] Stepping pH = 10.23
[50:38] Dispensed 0.000094 mL of Base (0.5 M KOH)
[50:43] Stepping pH = 10.24
[50:58] Stirrer speed set to 0
[51:08] Datapoint id 52 collected
[51:08] Charge balance equation is out by 39.5%
[51:08] Stirrer speed set to 55
[51:13] pH 10.24 -> 10.44
[51:13] Using cautious pH adjust
[51:13] Dispensed 0.000729 mL of Base (0.5 M KOH)
[51:19] Stepping pH = 10.36
[51:19] Dispensed 0.000376 mL of Base (0.5 M KOH)
[51:24] Stepping pH = 10.41
[51:24] Dispensed 0.000165 mL of Base (0.5 M KOH)
[51:29] Stepping pH = 10.43
[51:29] Dispensed 0.000071 mL of Base (0.5 M KOH)
[51:34] Stepping pH = 10.43
[51:49] Stirrer speed set to 0
[52:00] Datapoint id 53 collected
[52:00] Charge balance equation is out by 9.5%
[52:00] Stirrer speed set to 55
[52:05] pH 10.42 -> 10.62
[52:05] Using charge balance adjust
[52:05] Dispensed 0.001482 mL of Base (0.5 M KOH)
[52:25] Stirrer speed set to 0
[52:35] Datapoint id 54 collected
[52:35] Charge balance equation is out by -24.8%
[52:35] Stirrer speed set to 55
[52:40] pH 10.58 -> 10.78
[52:40] Using cautious pH adjust
[52:40] Dispensed 0.000823 mL of Base (0.5 M KOH)
[52:45] Stepping pH = 10.64
[52:46] Dispensed 0.001011 mL of Base (0.5 M KOH)

Sample name: **M16_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01009**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01009_M16_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 12:08:09 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[52:51] Stepping pH = 10.71
[52:51] Dispensed 0.000682 mL of Base (0.5 M KOH)
[52:56] Stepping pH = 10.76
[52:56] Dispensed 0.000259 mL of Base (0.5 M KOH)
[53:01] Stepping pH = 10.77
[53:16] Stirrer speed set to 0
[53:26] Datapoint id 55 collected
[53:26] Charge balance equation is out by -67.6%
[53:26] Stirrer speed set to 55
[53:31] pH 10.77 -> 10.97
[53:31] Using cautious pH adjust
[53:32] Dispensed 0.001058 mL of Base (0.5 M KOH)
[53:37] Stepping pH = 10.84
[53:37] Dispensed 0.001223 mL of Base (0.5 M KOH)
[53:42] Stepping pH = 10.91
[53:42] Dispensed 0.000682 mL of Base (0.5 M KOH)
[53:47] Stepping pH = 10.96
[53:47] Dispensed 0.000165 mL of Base (0.5 M KOH)
[53:52] Stepping pH = 10.96
[54:07] Stirrer speed set to 0
[54:17] Datapoint id 56 collected
[54:17] Charge balance equation is out by -47.4%
[54:17] Stirrer speed set to 55
[54:22] pH 10.96 -> 11.16
[54:22] Using cautious pH adjust
[54:23] Dispensed 0.001482 mL of Base (0.5 M KOH)
[54:28] Stepping pH = 11.04
[54:28] Dispensed 0.001458 mL of Base (0.5 M KOH)
[54:33] Stepping pH = 11.11
[54:33] Dispensed 0.000847 mL of Base (0.5 M KOH)
[54:38] Stepping pH = 11.14
[54:38] Dispensed 0.000329 mL of Base (0.5 M KOH)
[54:43] Stepping pH = 11.15
[54:58] Stirrer speed set to 0
[55:08] Datapoint id 57 collected
[55:08] Charge balance equation is out by -38.3%
[55:08] Stirrer speed set to 55
[55:14] pH 11.15 -> 11.35
[55:14] Using cautious pH adjust
[55:14] Dispensed 0.002234 mL of Base (0.5 M KOH)
[55:19] Stepping pH = 11.23
[55:19] Dispensed 0.002258 mL of Base (0.5 M KOH)
[55:24] Stepping pH = 11.31
[55:24] Dispensed 0.001058 mL of Base (0.5 M KOH)
[55:29] Stepping pH = 11.34
[55:44] Stirrer speed set to 0
[55:54] Datapoint id 58 collected
[55:54] Charge balance equation is out by -24.3%
[55:54] Stirrer speed set to 55
[55:59] pH 11.34 -> 11.54
[55:59] Using cautious pH adjust
[56:00] Dispensed 0.003434 mL of Base (0.5 M KOH)
[56:05] Stepping pH = 11.44
[56:05] Dispensed 0.002775 mL of Base (0.5 M KOH)
[56:10] Stepping pH = 11.50
[56:10] Dispensed 0.001364 mL of Base (0.5 M KOH)
[56:15] Stepping pH = 11.53
[56:30] Stirrer speed set to 0
[56:40] Datapoint id 59 collected

Sample name: **M16_octanol** Experiment start time: **3/1/2018 12:08:09 PM**
Assay name: **pH-metric high logP** Analyst: **Pion**
Assay ID: **18C-01009** Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01009_M16_octanol_pH-metric high logP.t3r**

Experiment Log (continued)

[56:40] Charge balance equation is out by -10.4%
[56:40] Stirrer speed set to 55
[56:45] pH 11.54 -> 11.74
[56:45] Using charge balance adjust
[56:46] Dispensed 0.010748 mL of Base (0.5 M KOH)
[57:06] Stirrer speed set to 0
[57:16] Datapoint id 60 collected
[57:16] Charge balance equation is out by -12.6%
[57:16] Stirrer speed set to 55
[57:21] pH 11.71 -> 11.91
[57:21] Using charge balance adjust
[57:22] Dispensed 0.016345 mL of Base (0.5 M KOH)
[57:42] Stirrer speed set to 0
[57:52] Datapoint id 61 collected
[57:52] Charge balance equation is out by -9.7%
[57:52] Stirrer speed set to 55
[57:57] pH 11.90 -> 12.05
[57:57] Using charge balance adjust
[57:58] Dispensed 0.018156 mL of Base (0.5 M KOH)
[58:18] Stirrer speed set to 0
[58:28] Datapoint id 62 collected
[58:28] Charge balance equation is out by -33.1%
[58:28] Titration 3 of 3
[58:28] Adding initial titrants
[58:28] Automatically add 0.30000 mL of Octanol
[58:35] Dispensed 0.300000 mL of Octanol
[58:35] Stirrer speed set to 10
[58:36] Stirrer speed set to 60
[58:36] Iterative adjust 12.04 -> 2.00
[58:36] pH 12.04 -> 2.00
[58:38] Dispensed 0.100000 mL of Acid (0.5 M HCl)
[58:44] pH 2.47 -> 2.00
[58:45] Dispensed 0.037465 mL of Acid (0.5 M HCl)
[58:50] pH 2.03 -> 2.00
[58:50] Dispensed 0.003904 mL of Acid (0.5 M HCl)
[59:40] Stirrer speed set to 0
[59:50] Datapoint id 63 collected
[59:50] Stirrer speed set to 60
[59:55] pH 1.98 -> 2.18
[59:55] Using cautious pH adjust
[59:56] Dispensed 0.011265 mL of Base (0.5 M KOH)
[1:00:01] Stepping pH = 2.06
[1:00:01] Dispensed 0.008796 mL of Base (0.5 M KOH)
[1:00:06] Stepping pH = 2.15
[1:00:06] Dispensed 0.001881 mL of Base (0.5 M KOH)
[1:00:11] Stepping pH = 2.18
[1:00:26] Stirrer speed set to 0
[1:00:47] Datapoint id 64 collected
[1:00:47] Charge balance equation is out by 2.6%
[1:00:47] Stirrer speed set to 60
[1:00:52] pH 2.19 -> 2.39
[1:00:52] Using charge balance adjust
[1:00:52] Dispensed 0.013805 mL of Base (0.5 M KOH)
[1:01:12] Stirrer speed set to 0
[1:01:22] Datapoint id 65 collected
[1:01:22] Charge balance equation is out by -4.3%
[1:01:22] Stirrer speed set to 60
[1:01:27] pH 2.39 -> 2.59
[1:01:27] Using charge balance adjust

Sample name: **M16_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01009**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01009_M16_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 12:08:09 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:01:28] Dispensed 0.008866 mL of Base (0.5 M KOH)
[1:01:48] Stirrer speed set to 0
[1:01:58] Datapoint id 66 collected
[1:01:58] Charge balance equation is out by -13.7%
[1:01:58] Stirrer speed set to 60
[1:02:03] pH 2.57 -> 2.77
[1:02:03] Using charge balance adjust
[1:02:03] Dispensed 0.006021 mL of Base (0.5 M KOH)
[1:02:23] Stirrer speed set to 0
[1:02:34] Datapoint id 67 collected
[1:02:34] Charge balance equation is out by -21.7%
[1:02:34] Stirrer speed set to 60
[1:02:39] pH 2.73 -> 2.93
[1:02:39] Using cautious pH adjust
[1:02:39] Dispensed 0.002187 mL of Base (0.5 M KOH)
[1:02:44] Stepping pH = 2.82
[1:02:44] Dispensed 0.001834 mL of Base (0.5 M KOH)
[1:02:49] Stepping pH = 2.89
[1:02:49] Dispensed 0.000753 mL of Base (0.5 M KOH)
[1:02:54] Stepping pH = 2.92
[1:03:09] Stirrer speed set to 0
[1:03:27] Datapoint id 68 collected
[1:03:27] Charge balance equation is out by -9.5%
[1:03:27] Stirrer speed set to 60
[1:03:33] pH 2.93 -> 3.13
[1:03:33] Using charge balance adjust
[1:03:33] Dispensed 0.003175 mL of Base (0.5 M KOH)
[1:03:53] Stirrer speed set to 0
[1:04:03] Datapoint id 69 collected
[1:04:03] Charge balance equation is out by -12.8%
[1:04:03] Stirrer speed set to 60
[1:04:09] pH 3.11 -> 3.31
[1:04:09] Using charge balance adjust
[1:04:09] Dispensed 0.002587 mL of Base (0.5 M KOH)
[1:04:29] Stirrer speed set to 0
[1:04:40] Datapoint id 70 collected
[1:04:40] Charge balance equation is out by 10.9%
[1:04:40] Stirrer speed set to 60
[1:04:45] pH 3.34 -> 3.54
[1:04:45] Using charge balance adjust
[1:04:45] Dispensed 0.002305 mL of Base (0.5 M KOH)
[1:05:05] Stirrer speed set to 0
[1:05:15] Datapoint id 71 collected
[1:05:15] Charge balance equation is out by 48.3%
[1:05:15] Stirrer speed set to 60
[1:05:20] pH 3.64 -> 3.84
[1:05:20] Using cautious pH adjust
[1:05:20] Dispensed 0.001152 mL of Base (0.5 M KOH)
[1:05:25] Stepping pH = 3.89
[1:05:40] Stirrer speed set to 0
[1:05:51] Datapoint id 72 collected
[1:05:51] Charge balance equation is out by 50.0%
[1:05:51] Stirrer speed set to 60
[1:05:56] pH 3.89 -> 4.09
[1:05:56] Using cautious pH adjust
[1:05:56] Dispensed 0.001105 mL of Base (0.5 M KOH)
[1:06:01] Stepping pH = 4.44
[1:06:16] Stirrer speed set to 0
[1:06:26] Datapoint id 73 collected

Sample name: **M16_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01009**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01009_M16_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 12:08:09 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:06:26] Charge balance equation is out by 50.0%
[1:06:26] Stirrer speed set to 60
[1:06:32] pH 4.44 -> 4.64
[1:06:32] Using cautious pH adjust
[1:06:32] Dispensed 0.000706 mL of Base (0.5 M KOH)
[1:06:37] Stepping pH = 6.57
[1:06:52] Stirrer speed set to 0
[1:07:47] Datapoint id 74 collected
[1:07:47] Charge balance equation is out by 50.0%
[1:07:47] Stirrer speed set to 60
[1:07:53] pH 6.31 -> 6.51
[1:07:53] Using cautious pH adjust
[1:07:53] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:07:58] Stepping pH = 6.28
[1:07:58] Dispensed 0.000235 mL of Base (0.5 M KOH)
[1:08:03] Stepping pH = 8.21
[1:08:18] Stirrer speed set to 0
[1:09:18] Datapoint id 75 collected
[1:09:18] Charge balance equation is out by -228.6%
[1:09:18] Stirrer speed set to 60
[1:09:23] pH 7.81 -> 8.01
[1:09:23] Using cautious pH adjust
[1:09:23] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:09:28] Stepping pH = 7.85
[1:09:28] Dispensed 0.000094 mL of Base (0.5 M KOH)
[1:09:33] Stepping pH = 8.33
[1:09:48] Stirrer speed set to 0
[1:10:33] Datapoint id 76 collected
[1:10:33] Charge balance equation is out by -40.8%
[1:10:33] Stirrer speed set to 60
[1:10:38] pH 8.20 -> 8.40
[1:10:38] Using cautious pH adjust
[1:10:38] Dispensed 0.000118 mL of Base (0.5 M KOH)
[1:10:43] Stepping pH = 8.56
[1:10:58] Stirrer speed set to 0
[1:11:21] Datapoint id 77 collected
[1:11:21] Charge balance equation is out by 50.0%
[1:11:21] Stirrer speed set to 60
[1:11:26] pH 8.49 -> 8.69
[1:11:26] Using cautious pH adjust
[1:11:26] Dispensed 0.000188 mL of Base (0.5 M KOH)
[1:11:31] Stepping pH = 8.91
[1:11:46] Stirrer speed set to 0
[1:11:58] Datapoint id 78 collected
[1:11:58] Charge balance equation is out by 50.0%
[1:11:58] Stirrer speed set to 60
[1:12:03] pH 8.87 -> 9.07
[1:12:03] Using cautious pH adjust
[1:12:03] Dispensed 0.000400 mL of Base (0.5 M KOH)
[1:12:09] Stepping pH = 9.33
[1:12:24] Stirrer speed set to 0
[1:12:35] Datapoint id 79 collected
[1:12:35] Charge balance equation is out by 50.0%
[1:12:35] Stirrer speed set to 60
[1:12:40] pH 9.30 -> 9.50
[1:12:40] Using cautious pH adjust
[1:12:40] Dispensed 0.000800 mL of Base (0.5 M KOH)
[1:12:45] Stepping pH = 9.79
[1:13:00] Stirrer speed set to 0

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Experiment start time: **3/1/2018 12:08:09 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:13:10] Datapoint id 80 collected
[1:13:10] Charge balance equation is out by 50.0%
[1:13:10] Stirrer speed set to 60
[1:13:15] pH 9.77 -> 9.97
[1:13:15] Using cautious pH adjust
[1:13:15] Dispensed 0.001105 mL of Base (0.5 M KOH)
[1:13:20] Stepping pH = 10.15
[1:13:36] Stirrer speed set to 0
[1:13:46] Datapoint id 81 collected
[1:13:46] Charge balance equation is out by 50.0%
[1:13:46] Stirrer speed set to 60
[1:13:51] pH 10.14 -> 10.34
[1:13:51] Using cautious pH adjust
[1:13:51] Dispensed 0.001082 mL of Base (0.5 M KOH)
[1:13:56] Stepping pH = 10.37
[1:14:11] Stirrer speed set to 0
[1:14:21] Datapoint id 82 collected
[1:14:21] Charge balance equation is out by 50.0%
[1:14:21] Stirrer speed set to 60
[1:14:26] pH 10.36 -> 10.56
[1:14:26] Using cautious pH adjust
[1:14:26] Dispensed 0.001058 mL of Base (0.5 M KOH)
[1:14:31] Stepping pH = 10.51
[1:14:31] Dispensed 0.000306 mL of Base (0.5 M KOH)
[1:14:37] Stepping pH = 10.55
[1:14:37] Dispensed 0.000118 mL of Base (0.5 M KOH)
[1:14:42] Stepping pH = 10.55
[1:14:57] Stirrer speed set to 0
[1:15:07] Datapoint id 83 collected
[1:15:07] Charge balance equation is out by 29.7%
[1:15:07] Stirrer speed set to 60
[1:15:12] pH 10.55 -> 10.75
[1:15:12] Using cautious pH adjust
[1:15:12] Dispensed 0.001105 mL of Base (0.5 M KOH)
[1:15:17] Stepping pH = 10.66
[1:15:17] Dispensed 0.000682 mL of Base (0.5 M KOH)
[1:15:22] Stepping pH = 10.71
[1:15:22] Dispensed 0.000329 mL of Base (0.5 M KOH)
[1:15:27] Stepping pH = 10.73
[1:15:28] Dispensed 0.000188 mL of Base (0.5 M KOH)
[1:15:33] Stepping pH = 10.74
[1:15:48] Stirrer speed set to 0
[1:15:58] Datapoint id 84 collected
[1:15:58] Charge balance equation is out by -4.8%
[1:15:58] Stirrer speed set to 60
[1:16:03] pH 10.74 -> 10.94
[1:16:03] Using charge balance adjust
[1:16:03] Dispensed 0.002611 mL of Base (0.5 M KOH)
[1:16:23] Stirrer speed set to 0
[1:16:33] Datapoint id 85 collected
[1:16:33] Charge balance equation is out by -12.8%
[1:16:33] Stirrer speed set to 60
[1:16:38] pH 10.92 -> 11.12
[1:16:38] Using charge balance adjust
[1:16:39] Dispensed 0.003387 mL of Base (0.5 M KOH)
[1:16:59] Stirrer speed set to 0
[1:17:09] Datapoint id 86 collected
[1:17:09] Charge balance equation is out by -11.7%
[1:17:09] Stirrer speed set to 60

Sample name: **M16_octanol**
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Experiment start time: **3/1/2018 12:08:09 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:17:14] pH 11.10 -> 11.30
[1:17:14] Using charge balance adjust
[1:17:14] Dispensed 0.004751 mL of Base (0.5 M KOH)
[1:17:34] Stirrer speed set to 0
[1:17:44] Datapoint id 87 collected
[1:17:44] Charge balance equation is out by -27.1%
[1:17:44] Stirrer speed set to 60
[1:17:50] pH 11.25 -> 11.45
[1:17:50] Using cautious pH adjust
[1:17:50] Dispensed 0.003269 mL of Base (0.5 M KOH)
[1:17:55] Stepping pH = 11.34
[1:17:55] Dispensed 0.002893 mL of Base (0.5 M KOH)
[1:18:00] Stepping pH = 11.41
[1:18:00] Dispensed 0.001364 mL of Base (0.5 M KOH)
[1:18:05] Stepping pH = 11.44
[1:18:05] Dispensed 0.000470 mL of Base (0.5 M KOH)
[1:18:10] Stepping pH = 11.45
[1:18:26] Stirrer speed set to 0
[1:18:36] Datapoint id 88 collected
[1:18:36] Charge balance equation is out by -22.0%
[1:18:36] Stirrer speed set to 60
[1:18:41] pH 11.45 -> 11.65
[1:18:41] Using cautious pH adjust
[1:18:41] Dispensed 0.005103 mL of Base (0.5 M KOH)
[1:18:46] Stepping pH = 11.54
[1:18:46] Dispensed 0.004163 mL of Base (0.5 M KOH)
[1:18:51] Stepping pH = 11.61
[1:18:51] Dispensed 0.002023 mL of Base (0.5 M KOH)
[1:18:57] Stepping pH = 11.64
[1:19:12] Stirrer speed set to 0
[1:19:34] Datapoint id 89 collected
[1:19:34] Charge balance equation is out by -10.3%
[1:19:34] Stirrer speed set to 60
[1:19:39] pH 11.64 -> 11.84
[1:19:39] Using charge balance adjust
[1:19:40] Dispensed 0.015851 mL of Base (0.5 M KOH)
[1:20:00] Stirrer speed set to 0
[1:20:10] Datapoint id 90 collected
[1:20:10] Charge balance equation is out by -12.5%
[1:20:10] Stirrer speed set to 60
[1:20:15] pH 11.82 -> 12.02
[1:20:15] Using charge balance adjust
[1:20:16] Dispensed 0.024506 mL of Base (0.5 M KOH)
[1:20:36] Stirrer speed set to 0
[1:20:46] Datapoint id 91 collected
[1:20:46] Charge balance equation is out by -12.2%
[1:20:46] Stirrer speed set to 60
[1:20:51] pH 12.01 -> 12.05
[1:20:51] Using charge balance adjust
[1:20:51] Dispensed 0.007103 mL of Base (0.5 M KOH)
[1:21:12] Stirrer speed set to 0
[1:21:22] Datapoint id 92 collected
[1:21:22] Charge balance equation is out by -85.4%
[1:21:22] Argon flow rate set to 0
[1:21:26] Titrator arm moved over Titration position